

EAST UPDATE 09/811,359

L Number	Hits	Search Text	DB	Time stamp
1	2343	((544/333) or (544/277)).CCLS.	USPAT; US-PGPUB	2004/02/21 15:39
2	1916	(((544/333) or (544/277)).CCLS.) and (phenyl or naphthyl)	USPAT; US-PGPUB	2004/02/21 15:40
3	1861	(((544/333) or (544/277)).CCLS.) and (phenyl or naphthyl)) and (amino or alkoxy)	USPAT; US-PGPUB	2004/02/21 15:41
4	198	(((544/333) or (544/277)).CCLS.) and (phenyl or naphthyl)) and (amino or alkoxy)) and ('CRF' or anxiety)	USPAT; US-PGPUB	2004/02/21 15:41

09/ 811,359

Connecting via Winsock to STN

Welcome to STN International! Enter x:x

LOGINID:ssspta1202txn

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

\* \* \* \* \* Welcome to STN International \* \* \* \* \*

NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	SEP 09	CA/Caplus records now contain indexing from 1907 to the present
NEWS 4	DEC 08	INPADOC: Legal Status data reloaded
NEWS 5	SEP 29	DISSABS now available on STN
NEWS 6	OCT 10	PCTFULL: Two new display fields added
NEWS 7	OCT 21	BIOSIS file reloaded and enhanced
NEWS 8	OCT 28	BIOSIS file segment of TOXCENTER reloaded and enhanced
NEWS 9	NOV 24	MSDS-CCOHS file reloaded
NEWS 10	DEC 08	CABA reloaded with left truncation
NEWS 11	DEC 08	IMS file names changed
NEWS 12	DEC 09	Experimental property data collected by CAS now available in REGISTRY
NEWS 13	DEC 09	STN Entry Date available for display in REGISTRY and CA/Caplus
NEWS 14	DEC 17	DGENE: Two new display fields added
NEWS 15	DEC 18	BIOTECHNO no longer updated
NEWS 16	DEC 19	CROPU no longer updated; subscriber discount no longer available
NEWS 17	DEC 22	Additional INPI reactions and pre-1907 documents added to CAS databases
NEWS 18	DEC 22	IFIPAT/IFIUDB/IFICDB reloaded with new data and search fields
NEWS 19	DEC 22	ABI-INFORM now available on STN
NEWS 20	JAN 27	Source of Registration (SR) information in REGISTRY updated and searchable
NEWS 21	JAN 27	A new search aid, the Company Name Thesaurus, available in CA/Caplus
NEWS 22	FEB 05	German (DE) application and patent publication number format changes
NEWS EXPRESS	DECEMBER 28 CURRENT WINDOWS VERSION IS V7.00, CURRENT MACINTOSH VERSION IS V6.0b(ENG) AND V6.0Jb(JP), AND CURRENT DISCOVER FILE IS DATED 23 SEPTEMBER 2003	
NEWS HOURS	STN Operating Hours Plus Help Desk Availability	
NEWS INTER	General Internet Information	
NEWS LOGIN	Welcome Banner and News Items	
NEWS PHONE	Direct Dial and Telecommunication Network Access to STN	
NEWS WWW	CAS World Wide Web Site (general information)	

Enter NEWS followed by the item number or name to see news on that specific topic.

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\* \* \* \* \* STN Columbus \* \* \* \* \*

FILE 'HOME' ENTERED AT 10:41:35 ON 21 FEB 2004

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

0.21

0.21

FILE 'REGISTRY' ENTERED AT 10:41:51 ON 21 FEB 2004

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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Property values tagged with IC are from the ZIC/VINITI data file  
provided by InfoChem.

STRUCTURE FILE UPDATES: 19 FEB 2004 HIGHEST RN 652129-06-1

DICTIONARY FILE UPDATES: 19 FEB 2004 HIGHEST RN 652129-06-1

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

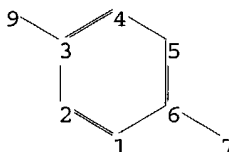
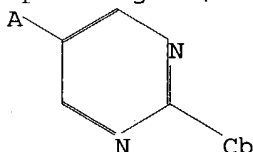
Please note that search-term pricing does apply when  
conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more  
information enter HELP PROP at an arrow prompt in the file or refer  
to the file summary sheet on the web at:  
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=>

Uploading C:\STNEXP4\QUERIES\09811359.str



chain nodes :

7 9

ring nodes :

1 2 3 4 5 6

chain bonds :

3-9 6-7

ring bonds :

1-2 1-6 2-3 3-4 4-5 5-6

exact/norm bonds :

3-9

exact bonds :

6-7

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 9:CLASS

Generic attributes :

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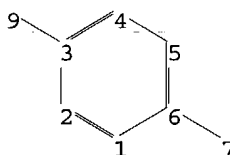
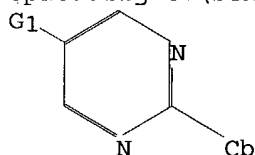
7:  
Saturation : Unsaturated

Element Count :  
Node 7: Limited  
C,C6-12

L1 STRUCTURE UPLOADED

=>

Uploading C:\STNEXP4\QUERIES\09811359a.str



chain nodes :  
7 9  
ring nodes :  
1 2 3 4 5 6  
chain bonds :  
3-9 6-7  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
3-9  
exact bonds :  
6-7  
normalized bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
isolated ring systems :  
containing 1 :

G1:O,N

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 9:CLASS  
Generic attributes :  
7:  
Saturation : Unsaturated

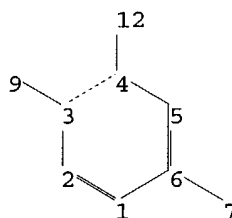
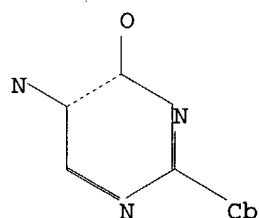
Element Count :  
Node 7: Limited  
C,C6-12

L2 STRUCTURE UPLOADED

=>

Uploading C:\STNEXP4\QUERIES\09811359b.str

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chain nodes :  
7 9 12  
ring nodes :  
1 2 3 4 5 6  
chain bonds :  
3-9 4-12 6-7  
ring bonds :  
1-2 1-6 2-3 3-4 4-5 5-6  
exact/norm bonds :  
1-2 1-6 2-3 3-4 3-9 4-5 4-12 5-6  
exact bonds :  
6-7  
isolated ring systems :  
containing 1 :

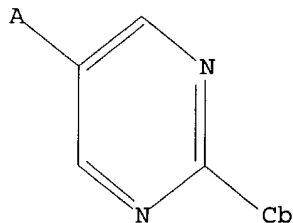
G1:O,N

Match level :  
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 9:CLASS 12:CLASS  
Generic attributes :  
7:  
Saturation : Unsaturated

Element Count :  
Node 7: Limited  
C,C6-12

L3 STRUCTURE UPLOADED

=> d l1  
L1 HAS NO ANSWERS  
L1 STR

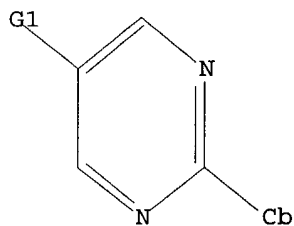


Structure attributes must be viewed using STN Express query preparation.

=> d l2

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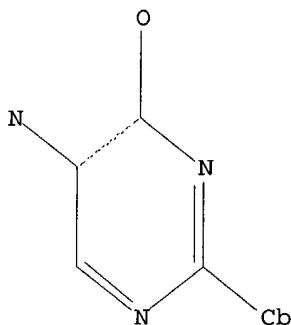
L2 HAS NO ANSWERS  
L2 STR



G1 O,N

Structure attributes must be viewed using STN Express query preparation.

=> d 13  
L3 HAS NO ANSWERS  
L3 STR



G1 O,N

Structure attributes must be viewed using STN Express query preparation.

=> s l1 ful  
FULL SEARCH INITIATED 10:44:15 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 683564 TO ITERATE

58.5% PROCESSED 400000 ITERATIONS  
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)  
SEARCH TIME: 00.00.11

8401 ANSWERS

FULL FILE PROJECTIONS: ONLINE \*\*INCOMPLETE\*\*  
BATCH \*\*INCOMPLETE\*\*  
PROJECTED ITERATIONS: 683564 TO 683564  
PROJECTED ANSWERS: 13997 TO 14715

L4 8401 SEA SSS FUL L1

=> s l2 ful  
FULL SEARCH INITIATED 10:44:36 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 118233 TO ITERATE

100.0% PROCESSED 118233 ITERATIONS  
SEARCH TIME: 00.00.05

5166 ANSWERS

09/ 811,359

L5 5166 SEA SSS FUL L2

=> s l3 ful

FULL SEARCH INITIATED 10:44:45 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 33355 TO ITERATE

100.0% PROCESSED 33355 ITERATIONS

316 ANSWERS

SEARCH TIME: 00.00.02

L6 316 SEA SSS FUL L3

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

467.10

467.31

FILE 'CAPLUS' ENTERED AT 10:45:05 ON 21 FEB 2004

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FILE COVERS 1907 - 21 Feb 2004 VOL 140 ISS 9

FILE LAST UPDATED: 20 Feb 2004 (20040220/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d his

(FILE 'HOME' ENTERED AT 10:41:35 ON 21 FEB 2004)

FILE 'REGISTRY' ENTERED AT 10:41:51 ON 21 FEB 2004

L1 STRUCTURE UPLOADED

L2 STRUCTURE UPLOADED

L3 STRUCTURE UPLOADED

L4 8401 S L1 FUL

L5 5166 S L2 FUL

L6 316 S L3 FUL

FILE 'CAPLUS' ENTERED AT 10:45:05 ON 21 FEB 2004

=> s l4 or l5

1421 L4

1099 L5

L7 1933 L4 OR L5

=> s l7 not (pyridyl or pyridin? or pyrimidin? or pyrimidyl or pyridazin? or thiophen?)

42729 PYRIDYL

249931 PYRIDIN?

76023 PYRIMIDIN?

2008 PYRIMIDYL

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13163 PYRIDAZIN?

57992 THIOPHEN?

L8 878 L7 NOT (PYRIDYL OR PYRIDIN? OR PYRIMIDIN? OR PYRIMIDYL OR PYRIDAZIN? OR THIOPHEN?)

=> s 18 and (phenyl or naphthyl)

309474 PHENYL

50268 NAPHTHYL

L9 81 L8 AND (PHENYL OR NAPHTHYL)

=> s 16

L10 68 L6

=> s 19 not 110

L11 74 L9 NOT L10

=> d 110 1- ibib abs fhitr

YOU HAVE REQUESTED DATA FROM 68 ANSWERS - CONTINUE? Y/(N):y

L10 ANSWER 1 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2004:20686 CAPLUS

DOCUMENT NUMBER: 140:77152

TITLE: Preparation of novel benzimidazole derivatives as neuropeptide Y receptor antagonists

INVENTOR(S): Otake, Norikazu; Moriya, Minoru; Ogino, Yoshio; Matsuda, Kenji; Nagae, Yoshikazu; Kanatani, Akio; Fukami, Takehiro

PATENT ASSIGNEE(S): Banyu Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 171 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

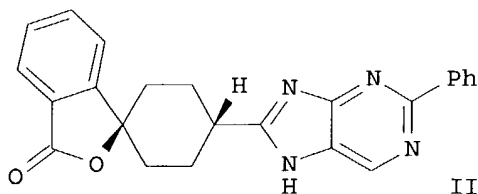
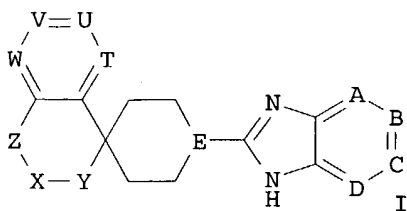
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004002986	A2	20040108	WO 2003-JP8161	20030626
W: AE, AG, AL, AM, AU, AZ, BA, BB, BR, BY, BZ, CA, CN, CO, CR, CU, DM, DZ, EC, GD, GH, HR, ID, IL, IN, IS, JP, KG, KR, KZ, LC, LK, LR, LT, LV, MA, MD, MG, MK, MN, MX, NI, NO, NZ, OM, PG, PH, PL, RU, SC, SG, SY, TJ, TM, TN, TT, UA, US, UZ, VC, VN, YU, ZA, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				

PRIORITY APPLN. INFO.: JP 2002-190978 A 20020628

OTHER SOURCE(S): MARPAT 140:77152

GI





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AB Benzimidazole derivs. of formula I [A, B, C, D = N, (substituted) CH; E = N, CH, C-OH; T, U, V, W = (substituted) CH, N; X = NSO<sub>2</sub>-alkyl, N-acyl, CO, etc.; Y = O, (substituted) NH, etc.; Z = (CH<sub>2</sub>)<sub>n</sub>; n = 0-1] are prepared as neuropeptide Y receptor antagonists. The compds. are useful in the treatment of bulimia, obesity or diabetes. Thus, II was prepared from trans-3'-oxospiro[cyclohexane-1,1'(3'H)-isobenzofuran]-4-carboxylic acid and 2-phenyl-4,5-diaminopyrimidine. II had IC<sub>50</sub> of 2.2 nM in neuropeptide Y binding inhibition test. Pharmaceutical compns. containing I are described.

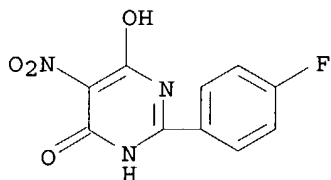
IT 640271-56-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of benzimidazole derivs. as neuropeptide Y receptor antagonists)

RN 640271-56-3 CAPLUS

CN 4(1H)-Pyrimidinone, 2-(4-fluorophenyl)-6-hydroxy-5-nitro- (9CI) (CA INDEX NAME)



L10 ANSWER 2 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:570644 CAPLUS

DOCUMENT NUMBER: 139:133575

TITLE: Preparation of bicyclic pyrimidinyl derivatives as adenosine receptor ligands

INVENTOR(S): Castelhana, Arlindo L.; McKibben, Bryan

PATENT ASSIGNEE(S): OSI Pharmaceuticals Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 105 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

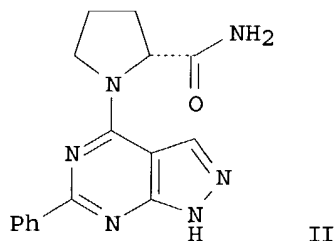
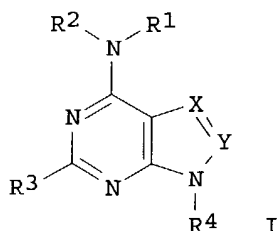
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003139427	A1	20030724	US 2002-227378	20020823
PRIORITY APPLN. INFO.:			US 2002-227378	20020823
OTHER SOURCE(S):		MARPAT 139:133575		

GI



AB Title compds. I [Y = N, CR5 and X = N, CR6 wherein X, Y are both N or when

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Y = CR5, X = N or when X = CR6, Y = N; R1-2 = H, alkoxy, aminoalkyl, etc; R3-4 = H, alkyl, aryl, alkylaryl] are prepared For instance, 3-amino-4-carbamoylpyrazole is acylated with benzoyl chloride (Pyridine, 50°, 5-6 h), cyclized to the corresponding pyrazolopyrimidine (water, K2CO3, 100°, 16 h), converted to the chloride (POCl3, 106°, 2 h) and used for reactions with various amines to give the example compds., e.g., II. II has Ki = 76.7 nM for the adenosine A1 receptor, Ki = 242.7 nM for A2a and Ki = 1480.5 nM for A2b. I are useful for the treatment of.

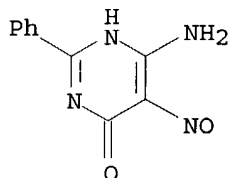
IT **5466-66-0P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of bicyclic pyrazolo- imidazo- and triazolopyrimidinyl derivs. as adenosine receptor ligands)

RN 5466-66-0 CAPLUS

CN 4(1H)-Pyrimidinone, 6-amino-5-nitroso-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 3 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:521326 CAPLUS

DOCUMENT NUMBER: 139:239663

TITLE: 2-Aryl-3,6-dialkyl-5-dialkylaminopyrimidin-4-ones as novel CRF-1 receptor antagonists

AUTHOR(S): Hodgetts, Kevin J.; Yoon, Taeyoung; Huang, Jianhua; Gulianello, Michael; Kieltyka, Andrzej; Primus, Renee; Brodbeck, Robbin; De Lombaert, Stephane; Doller, Dario

CORPORATE SOURCE: Neurogen Corporation, Branford, CT, 06405, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2003), 13(15), 2497-2500

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier Science B.V.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The discovery, synthesis and structure-activity studies of a novel series of 2-arylpyrimidin-4-ones as CRF-1 receptor antagonists is described. These compds. are structurally simple and display appropriate phys. properties for CNS agents.

IT **391936-44-0P**

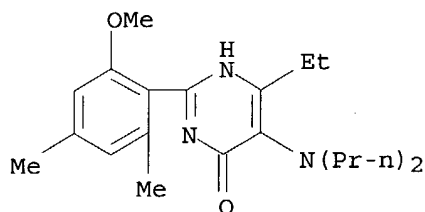
RL: PAC (Pharmacological activity); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation, phys. properties, and biol. activity of 2-aryl-3,6-dialkyl-5-dialkylaminopyrimidin-4-ones as novel CRF-1 receptor antagonists)

RN 391936-44-0 CAPLUS

CN 4(1H)-Pyrimidinone, 5-(dipropylamino)-6-ethyl-2-(2-methoxy-4,6-dimethylphenyl)- (9CI) (CA INDEX NAME)

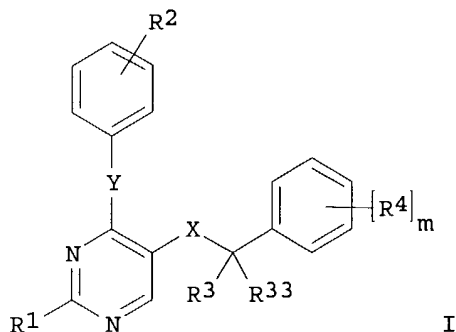
09/ 811,359



REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 4 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2002:408655 CAPLUS  
DOCUMENT NUMBER: 137:6189  
TITLE: Preparation of pyrimidine derivatives as NK1 antagonists  
INVENTOR(S): Stadler, Heinz  
PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.  
SOURCE: PCT Int. Appl., 55 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002042280	A2	20020530	WO 2001-EP13084	20011113
WO 2002042280	A3	20020822		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
US 2002099207	A1	20020725	US 2001-977586	20011015
AU 2002027921	A5	20020603	AU 2002-27921	20011113
EP 1339698	A2	20030903	EP 2001-989463	20011113
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR			
BR 2001015480	A	20031021	BR 2001-15480	20011113
NO 2003002291	A	20030521	NO 2003-2291	20030521
PRIORITY APPLN. INFO.:			EP 2000-125529 A	20001122
			WO 2001-EP13084 W	20011113
OTHER SOURCE(S):	MARPAT 137:6189			
GI				



AB The title compds. [I; R1 = alkyl, alkoxy, pyridinyl, pyrimidinyl, etc.; R2 = H, alkyl, alkoxy, halo, CF<sub>3</sub>; R3, R33 = H, alkyl; R4 = halo, CF<sub>3</sub>, alkoxy; R5 = H, alkyl; X = CONR, NRCO; Y = O, S, SO<sub>2</sub>, NR; m = 0-2] which have a good affinity to the NK1 receptor and therefore are suitable in the treatment of diseases, related to this receptor, were prepared and formulated. Thus, reacting 4-chloro-2-methylsulfanylpurimidine-5-carboxylic acid Et ester with o-cresol in the presence of Cs<sub>2</sub>CO<sub>3</sub> in MeCN (99%) followed by saponification (47%), and amidation of the resulting acid with [3,5-bis(trifluoromethyl)benzyl]methylamine (96%) afforded I [R1 = SMe; R2 = 2-Me; R3, R33 = H; R4 = 3,5-(CF<sub>3</sub>)<sub>2</sub>; Y = O; X = CONMe] which showed pK<sub>i</sub> of 7.38 against NK-1 receptor binding.

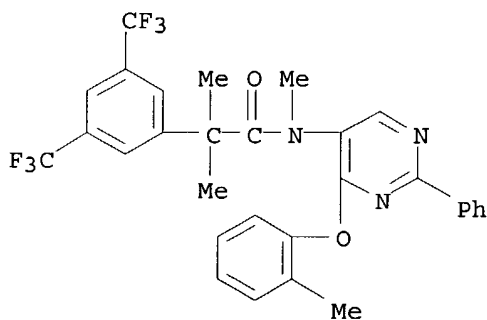
IT 432521-49-8P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of pyrimidine derivs. as NK1 antagonists)

RN 432521-49-8 CAPLUS

CN Benzeneacetamide, N,α,α-trimethyl-N-[4-(2-methylphenoxy)-2-phenyl-5-pyrimidinyl]-3,5-bis(trifluoromethyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 5 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:72057 CAPLUS

DOCUMENT NUMBER: 136:134771

TITLE: Preparation of 5-substituted 2-aryl-4-pyrimidinones as selective modulators of CRF 1 receptors

INVENTOR(S): Hodgetts, Kevin J.; Doller, Dario

PATENT ASSIGNEE(S): Neurogen Corporation, USA

SOURCE: PCT Int. Appl., 75 pp.

CODEN: PIXXD2

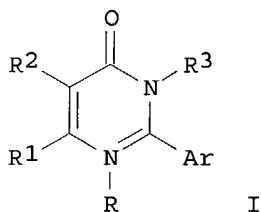
DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

## PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002006242	A2	20020124	WO 2001-US22513	20010718
WO 2002006242	A3	20020718		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2002052387	A1	20020502	US 2001-908444	20010718
EP 1301490	A2	20030416	EP 2001-958986	20010718
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2004504302	T2	20040212	JP 2002-512146	20010718
PRIORITY APPLN. INFO.:			US 2000-219703P	P 20000718
			WO 2001-US22513	W 20010718
OTHER SOURCE(S):		MARPAT 136:134771		
GI				



AB The title compds. [I; Ar = (un)substituted carbocyclic aryl, heteroaryl; R = O, Me, absent; R<sup>1</sup> = H, halo, CN, etc.; R<sup>2</sup> = alkyl, alkoxy, cycloalkyl, etc.; R<sup>3</sup> = H, alkyl, alkoxy, (di)alkylamino, etc.; provided that R<sup>1</sup> is not H, alkyl, or CF<sub>3</sub> when R<sup>2</sup> = H, alkyl, alkenyl] that act as selective modulators of CRF 1 receptors, and therefore are useful in the treatment of a number of CNS and peripheral disorders, particularly stress, anxiety, depression, cardiovascular disorders, and eating disorders, were prepared E.g., a multi-step synthesis of I [Ar = 2-MeO-4,6-Me<sub>2</sub>C<sub>6</sub>H<sub>2</sub>; R<sup>1</sup> = Me; R<sup>2</sup> = NPr<sub>2</sub>; R<sup>3</sup> = Me] was given. The exemplified compds. I showed IC<sub>50</sub> of ≤ 4 μM in assay for CRF1 receptor binding activity. Compds. I are also useful as probes for the localization of CRF receptors and as stds. in assays for CRF receptor binding. Methods of using the compds. I in receptor localization studies are given.

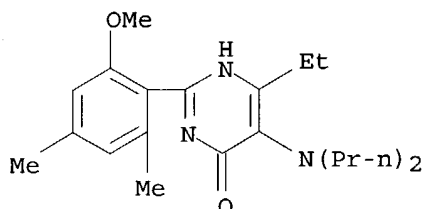
IT **391936-44-0P**

RL: DGN (Diagnostic use); PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of 5-substituted 2-aryl-4-pyrimidinones as selective modulators of CRF 1 receptors)

RN 391936-44-0 CAPLUS

CN 4(1H)-Pyrimidinone, 5-(dipropylamino)-6-ethyl-2-(2-methoxy-4,6-dimethylphenyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 6 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:693291 CAPLUS

DOCUMENT NUMBER: 135:242241

TITLE: 5-Substituted arylpyrimidines as selective modulators of CRF receptors

INVENTOR(S): Yoon, Taeyound; Delombaert, Stephane; Hodgetts, Kevin; Doller, Dario

PATENT ASSIGNEE(S): Neurogen Corporation, USA

SOURCE: PCT Int. Appl., 83 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001068614	A2	20010920	WO 2001-US8321	20010316
WO 2001068614	A3	20020606		
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CO, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 2002072521	A1	20020613	US 2001-811359	20010316
EP 1233949	A2	20020828	EP 2001-916687	20010316
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003527377	T2	20030916	JP 2001-567707	20010316
PRIORITY APPLN. INFO.:				
			US 2000-189774P	P 20000316
			US 2000-206454P	P 20000522
			WO 2001-US8321	W 20010316

OTHER SOURCE(S): MARPAT 135:242241

AB 2-Ar-4-R1-5-R2-6-R3pyrimidines (I, or a pharmaceutically acceptable salt thereof) are provided that can act as selective modulators of CRF receptors. In I: Ar is Ph, 1- or 2-naphthyl, each of which is mono, di, or trisubstituted or mono, di, or trisubstituted heteroaryl having from .apprx.5 to .apprx.7 ring members and 1 to .apprx.4 heteroatoms in the ring, the heteroatoms independently = N, O and S; R1 and R3 independently = H, halogen, cyano, nitro, alkyl, alkenyl, alkynyl, alkoxy, (cycloalkyl)alkyl, alkylthio, alkylsulfinyl, alkylsulfonyl, or mono- or dialkylcarboxamide, with the proviso that R1 and R3 are not both H; and R2 is alkyl, alkenyl, alkynyl, alkoxy, aminoalkyl, mono or dialkylamino, alkylthio, alkylsulfinyl, alkylsulfonyl, mono or dialkylcarboxamide, carbocyclic aryl or heteroaryl having from 1 to 3 rings, and 3 to 8 ring members in each ring and 1 to .apprx.3 heteroatoms. These compds. are useful in the treatment of a number of CNS and peripheral disorders, particularly stress, anxiety, depression, cardiovascular disorders, and

eating disorders. Methods of treatment of such disorders as well as packaged pharmaceutical compns. are also provided. Compds. of the invention are also useful as probes for the localization of CRF receptors and as stds. in assays for CRF receptor binding. Methods of using the compds. in receptor localization studies are given. Compds. of the invention do not exhibit activity as sodium ion channel blockers. They do exhibit in vitro t1/2 values of greater than 10 min and less than 4 h. MDCK toxicity was also measured. Six example preps. are included, but the methods of preparation are not claimed.

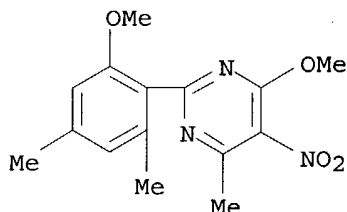
IT 360576-58-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of 5-substituted arylpyrimidines as selective modulators of CRF receptors)

RN 360576-58-5 CAPLUS

CN Pyrimidine, 4-methoxy-2-(2-methoxy-4,6-dimethylphenyl)-6-methyl-5-nitro-(9CI) (CA INDEX NAME)



L10 ANSWER 7 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:489401 CAPLUS

DOCUMENT NUMBER: 135:92657

TITLE: Preparation of 2-(2-alkoxy-5-sulfonylphenyl)-3H-imidazo[1,5-a][1,3,5]triazin-4-ones as inhibitors of cGMP metabolizing phosphodiesterases

INVENTOR(S): Niewoehner, Ulrich; Haning, Helmut; Lampe, Thomas; Es-Sayed, Mazen; Schmidt, Gunter; Bischoff, Erwin; Dembowski, Klaus; Perzborn, Elisabeth; Schlemmer, Karl-Heinz

PATENT ASSIGNEE(S): Bayer Aktiengesellschaft, Germany

SOURCE: PCT Int. Appl., 73 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: German

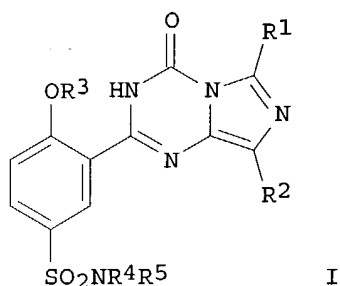
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001047928	A2	20010705	WO 2000-EP12597	20001212
WO 2001047928	A3	20020516		
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
DE 19962928	A1	20010628	DE 1999-19962928	19991224
DE 10003323	A1	20010802	DE 2000-10003323	20000127

09/ 811,359

EP 1244673            A2    20021002            EP 2000-993611    20001212  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR  
BR 2000017043        A    20030107            BR 2000-17043       20001212  
JP 2003519150        T2   20030617            JP 2001-549398      20001212  
US 2003195210        A1   20031016            US 2002-168194      20021104  
PRIORITY APPLN. INFO.:            DE 1999-19962928 A   19991224  
   DE 2000-10003323 A   20000127  
   WO 2000-EP12597    W   20001212  
OTHER SOURCE(S):            MARPAT 135:92657  
GI

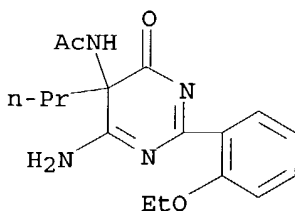


AB Title compds. [I; R1 = alkyl; R2 = alkyl, cycloalkyl; R3 = H, alkyl; R4, R5 = H, alkoxy, OH, (substituted) alkyl] were prepared as inhibitors of cGMP metabolizing phosphodiesterases (no data). Thus, 4-ethoxy-3-(6-methyl-4-oxo-8-propyl-3,4-dihydroimidazo[1,5-a][1,3,5]triazin-2-yl)benzenesulfonyl chloride (preparation given) in CH2Cl2 was stirred with N-(3,4-dimethoxyphenylethyl)-N-methylamine for 2 h at room temperature to give 98% N-[2-(3,4-dimethoxyphenyl)ethyl]-4-ethoxy-N-methyl-3-(6-methyl-4-oxo-8-propyl-3,4-dihydroimidazo[1,5-a][1,3,5]triazin-2-yl)benzenesulfonamide.

IT **346605-61-6P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of alkoxy sulfonyl phenylimidazotriazinones as inhibitors of cGMP metabolizing phosphodiesterases)

RN 346605-61-6 CAPLUS

CN Acetamide, N-[6-amino-2-(2-ethoxyphenyl)-4,5-dihydro-4-oxo-5-propyl-5-pyrimidinyl]- (9CI) (CA INDEX NAME)

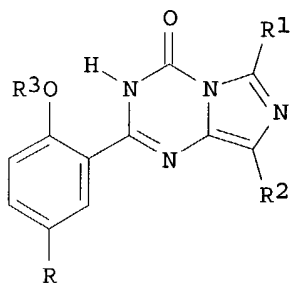


L10 ANSWER 8 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2001:479151 CAPLUS  
DOCUMENT NUMBER: 135:76905  
TITLE: Preparation of imidazotriazinones as cGMP PDE inhibitors  
INVENTOR(S): Niewoehner, Ulrich; Haning, Helmut; Lampe, Thomas;

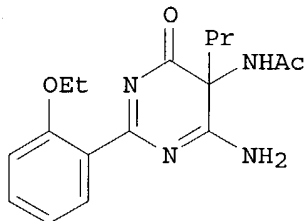


Es-Sayed, Mazen; Schmidt, Gunter; Bischoff, Erwin;  
 Dembowski, Klaus; Perzborn, Elisabeth; Schlemmer,  
 Karl-Heinz  
 PATENT ASSIGNEE(S): Bayer A.-G., Germany  
 SOURCE: Ger. Offen., 38 pp.  
 CODEN: GWXXBX  
 DOCUMENT TYPE: Patent  
 LANGUAGE: German  
 FAMILY ACC. NUM. COUNT: 2  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19962928	A1	20010628	DE 1999-19962928	19991224
WO 2001047928	A2	20010705	WO 2000-EP12597	20001212
WO 2001047928	A3	20020516		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1244673	A2	20021002	EP 2000-993611	20001212
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
BR 2000017043	A	20030107	BR 2000-17043	20001212
ZA 2002004457	A	20030604	ZA 2002-4457	20001212
JP 2003519150	T2	20030617	JP 2001-549398	20001212
PRIORITY APPLN. INFO.:				
			DE 1999-19962928 A	19991224
			DE 2000-10003323 A	20000127
			WO 2000-EP12597 W	20001212
OTHER SOURCE(S): MARPAT 135:76905				
GI				



I



II

AB Title compds. [I; R<sub>1</sub> = alkyl; R<sub>2</sub> = (cyclo)alkyl; R<sub>3</sub> = H or alkyl; R<sub>4</sub>, R<sub>5</sub> = H, (un)substituted alkyl, alkoxy, etc.; NR<sub>4</sub>R<sub>5</sub> = heterocyclyl] were prepared as cGMP PDE inhibitors (no data). Thus, 2-(EtO)C<sub>6</sub>H<sub>4</sub>C(:NH)NH<sub>2</sub>.HCl was cyclocondensed with PrC(CN)(NHAc)CO<sub>2</sub>Et (preparation each given) to give pyrimidinone II which was treated with Me<sub>3</sub>SiCl and the product refluxed with NH(SiMe<sub>3</sub>)<sub>3</sub> to give, after chlorosulfonation, I (R = SO<sub>2</sub>R<sub>6</sub>, R<sub>1</sub> = Me, R<sub>2</sub> = Pr, R<sub>3</sub> = Et)(III; R<sub>6</sub> = Cl). The latter was amidated by 1-(2-hydroxyethyl)piperazine to give III [R<sub>6</sub> = 4-(2-hydroxyethyl)-1-piperazinyl].

IT 346605-61-6P

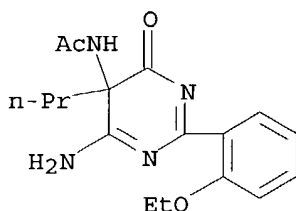
09/ 811,359

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)

(preparation of imidazotriazinones as cGMP PDE inhibitors)

RN 346605-61-6 CAPLUS

CN Acetamide, N-[6-amino-2-(2-ethoxyphenyl)-4,5-dihydro-4-oxo-5-propyl-5-pyrimidinyl]- (9CI) (CA INDEX NAME)



L10 ANSWER 9 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:279454 CAPLUS

DOCUMENT NUMBER: 134:295831

TITLE: Preparation of 2-(2-alkoxy-5-heterocyclylsulfonylphenyl)purin-6-ones as phosphodiesterase inhibitors

INVENTOR(S): Maw, Graham Nigel; Rawson, David James

PATENT ASSIGNEE(S): Pfizer Limited, UK; Pfizer Inc.

SOURCE: Eur. Pat. Appl., 44 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

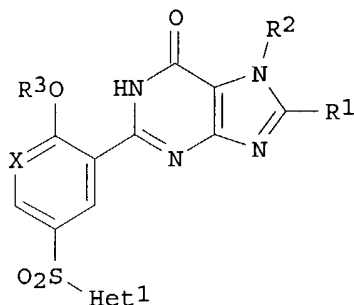
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1092718	A1	20010418	EP 2000-308644	20001002
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6440982	B1	20020827	US 2000-650848	20000829
JP 2001114782	A2	20010424	JP 2000-310665	20001011
BR 2000004786	A	20010522	BR 2000-4786	20001011
JP 2003128673	A2	20030508	JP 2002-224638	20001011
US 2003004173	A1	20030102	US 2002-189655	20020703
US 6593332	B2	20030715		
US 2003013727	A1	20030116	US 2002-189680	20020703
US 6586439	B2	20030701		

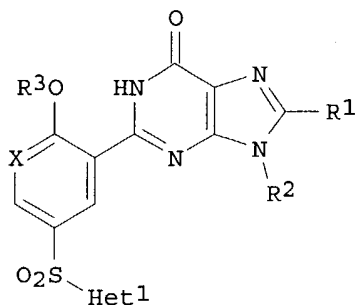
PRIORITY APPLN. INFO.: GB 1999-24020 A 19991011  
US 2000-650848 A3 20000829  
JP 2000-310665 A3 20001011

OTHER SOURCE(S): MARPAT 134:295831

GI



I



II

AB The title compds. [I or II; X = CH, N; R1 = H, CN, aryl, etc.; R2 = H, aryl, alkyl, etc.; R3 = H, (un)substituted alkyl; Het1 = 4-12 membered heterocyclyl which contains at least one N atom and, optionally, one or more further heteroatoms selected from N, O, and/or S], useful in the curative and prophylactic treatment of medical conditions for which inhibition of a cyclic guanosine 3',5'-monophosphate phosphodiesterase (e.g. cGMP PDE5) is desired (such as male erectile dysfunction), were prepared and formulated. E.g., 3-step synthesis of II [X = CH; R1 = H; R2, R3 = Pr; Het1 = 4-(pyridin-2-yl)piperazin-1-yl] which showed 100% PDE5 inhibition at 10 nM, was given.

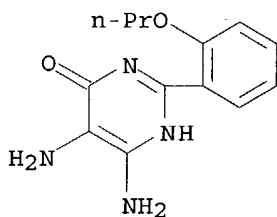
IT 57075-34-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of 2-(2-alkoxy-5-heterocyclylsulfonylphenyl)purin-6-ones as phosphodiesterase inhibitors)

RN 57075-34-0 CAPLUS

CN 4(1H)-Pyrimidinone, 5,6-diamino-2-(2-propoxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT:

9

THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 10 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:179819 CAPLUS

DOCUMENT NUMBER: 134:222726

TITLE: Preparation of phenyl purinone derivatives for the treatment of precancerous lesions

INVENTOR(S): Piazza, Gary A.; Pamukcu, Rifat

PATENT ASSIGNEE(S): Cell Pathways, Inc., USA

SOURCE: U.S., 31 pp., Cont. of U. S. Ser. No. 472,804.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

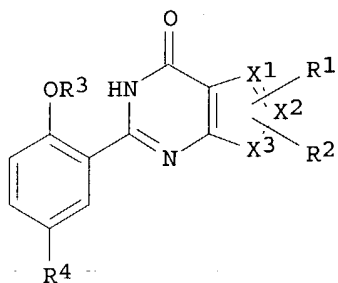
KIND DATE

APPLICATION NO. DATE

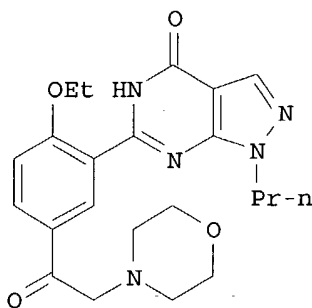
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09/ 811,359

US 6200980 B1 20010313 US 1997-842854 19970417  
PRIORITY APPLN. INFO.: US 1995-472804 A1 19950607  
OTHER SOURCE(S): MARPAT 134:222726  
GI



I



II

AB Title compds. (I) [wherein R1 = H, (fluoro)alkyl, or cycloalkyl; R2 = H, (fluoro)alkyl, or cycloalkylalkyl; R3 = (fluoro)alkyl, cycloalkyl(alkyl), alkenyl or alkynyl; R4 = halo or (un)substituted alkyl, alkenyl, alkanoyl, carbamoyl, carboxy, amino, sulfamoylamino, Ph, pyridyl, or imidazolyl, etc.; X1-X3 = independently N or C with the proviso that at least 2 of X1-X3 = N] were prepared for inhibiting the growth of neoplastic cells. For example, the 4H-pyrazolo[3,4-d]pyrimidin-4-one (II) was formed in a multi-step synthesis involving amidation of 5-amino-1-propylpyrazole-4-carboxamide with 2-ethoxybenzoyl chloride (74%), cyclization using aqueous NaOH (89%), acetylation with bromoacetyl bromide in the presence of AlCl3 (92%), and addition of morpholine in K2CO3 and MeCN (85%). In a cell growth inhibition assay examining the effects of I on human colon carcinoma cells, administration of 40  $\mu$ M of 2-(2-propoxyphenyl)-8-azapurin-6-one resulted in 30% apoptotic cells and 2% necrosis compared to 7% and 5%, resp., for the control. Pharmaceutical compns. for oral and parenteral administration of I are also included.

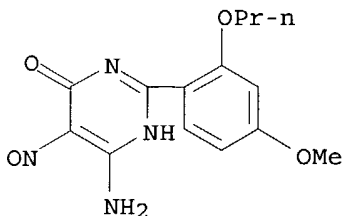
IT 127979-83-3P, 2-(4-Methoxy-2-propoxyphenyl)-4-amino-5-nitrosopyrimidin-6-one

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of Ph purinone derivs. for treatment of precancerous lesions)

RN 127979-83-3 CAPLUS

CN 4(1H)-Pyrimidinone, 6-amino-2-(4-methoxy-2-propoxyphenyl)-5-nitroso- (9CI)  
(CA INDEX NAME)

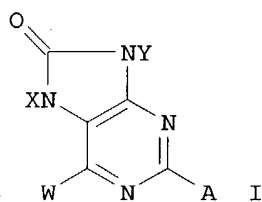


REFERENCE COUNT: 137 THERE ARE 137 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

09/ 811,359

DOCUMENT NUMBER: 134:173047  
TITLE: Pharmaceuticals containing 2-aryl-8-oxodihydropurines  
for anxiolytics and antidepressants  
INVENTOR(S): Murata, Akiya; Masumoto, Kaoru; Kondo, Masanori;  
Furukawa, Kiyoshi; Oka, Makoto  
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 36 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001048882	A2	20010220	JP 2000-165263	20000602
PRIORITY APPLN. INFO.:			JP 1999-154830	A 19990602
OTHER SOURCE(S):	MARPAT 134:173047			
GI				

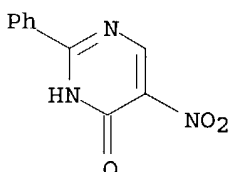


AB The pharmaceuticals contain dihydropurines I [W = H, lower alkyl, halo, lower alkoxy, amino, etc.; X = H, lower alkyl, (cycloalkyl)alkyl, phenylalkyl, CHR<sub>3</sub>CONR<sub>1</sub>R<sub>2</sub>, etc.; R<sub>1</sub> = lower alkyl, alkenyl, cycloalkyl, etc.; R<sub>2</sub> = lower alkyl, cycloalkyl, Ph, etc.; R<sub>3</sub> = H, lower alkyl, hydroxyalkyl; Y = H, lower alkyl, cycloalkyl, (cycloalkyl)alkyl, lower alkenyl, CHR<sub>3</sub>CONR<sub>1</sub>R<sub>2</sub>, etc.; A = (un)substituted Ph, heteroaryl; ≥1 group selected from X, Y is CHR<sub>3</sub>CONR<sub>1</sub>R<sub>2</sub>] or pharmaceutically acceptable acid salts. 7,9-Dihydro-9-methyl-2-phenyl-8H-purin-8-one (7.0 g) was reacted with 8.3 g 2-bromo-N-ethyl-N-phenylacetamide in the presence of NaH in DMF at room temperature for 3 h to give 10.3 g N-ethyl-8,9-dihydro-9-methyl-8-oxo-2-phenyl-N-phenyl-7H-purine-7-acetamide showing good antidepressant activity in rats.

IT 3749-46-0P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(pharmaceuticals containing aryloxodihydropurines for anxiolytics and antidepressants)

RN 3749-46-0 CAPLUS

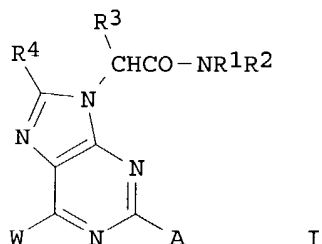
CN 4(1H)-Pyrimidinone, 5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



09/ 811,359

DOCUMENT NUMBER: 134:17498  
TITLE: Preparation of 2-arylpyrimidine-9-acetamide derivatives having selective action on peripheral benzodiazepine receptor, process for the preparation thereof, medicinal compositions containing the same and intermediates of the derivatives  
INVENTOR(S): Murata, Teruya; Kondo, Katsunori; Masumoto, Kaoru; Kohayakawa, Hitoshi; Furukawa, Kiyoshi  
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan  
SOURCE: PCT Int. Appl., 78 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

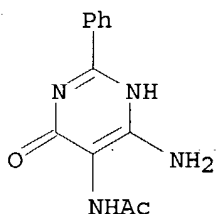
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000073306	A1	20001207	WO 2000-JP3374	20000526
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
JP 2003146987	A2	20030521	JP 1999-150878	19990531
PRIORITY APPLN. INFO.:			JP 1999-150878	A 19990531
OTHER SOURCE(S):		MARPAT 134:17498		
GI				



AB The title 2-arylpyrimidine-9-acetamide derivs. represented by general formula (I; R<sup>1</sup> is lower alkyl, cycloalkyl, cycloalkylated lower alkyl, or the like; R<sup>2</sup> is lower alkyl, substituted or unsubstituted Ph, or the like; R<sup>3</sup> is hydrogen or the like; R<sup>4</sup> is hydrogen, lower alkyl, cycloalkyl, halogeno, lower alkoxy, or the like; A is substituted or unsubstituted Ph or the like; W is hydrogen, lower alkyl, halogeno, lower alkoxy, lower alkylthio, lower alkanoyl, or the like) or pharmaceutically acceptable acid addition salts thereof are prepared as well as pharmaceutical compns. containing them. These compds. selectively act on peripheral benzodiazepine receptor BZ<sub>3</sub> receptor and are useful as therapeutic and preventive drugs for central nervous system diseases such as anxiety-related diseases, depression and epilepsy. Thus, a mixture of 2-(5-amino-2-phenyl-4-pyrimidinylamino)-N-methyl-N-phenylacetamide and DMF was heated at 180° with stirring for 2 h to give N-methyl-N-phenyl-2-phenyl-9H-purine-9-acetamide (II). II and N-methyl-N-phenyl-8-chloro-2-phenyl-9H-purine-9-acetamide inhibited the binding of [<sup>3</sup>H]4'-chlorodiazepam to BZ<sub>3</sub> receptor prepared from rat kidney with IC<sub>50</sub> of 0.88 and 0.23 nM,

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resp.  
IT 310408-58-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT  
(Reactant or reagent)  
(preparation of 2-arylpurine-9-acetamide derivs. having selective action on  
peripheral benzodiazepine receptor as drugs)  
RN 310408-58-3 CAPLUS  
CN Acetamide, N-(6-amino-1,4-dihydro-4-oxo-2-phenyl-5-pyrimidinyl)- (9CI)  
(CA INDEX NAME)

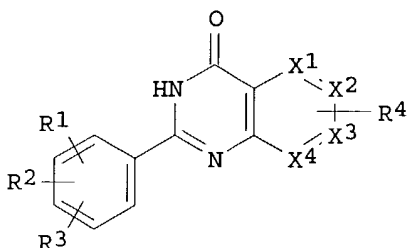


REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 13 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2000:304315 CAPLUS  
DOCUMENT NUMBER: 132:321870  
TITLE: Preparation of pyridopyrimidinones,  
pyrimidopyrimidinones, pyrimidotriazinones, and  
related compounds for the treatment of precancerous  
lesions.  
INVENTOR(S): Piazza, Gary A.; Pamukcu, Rifat  
PATENT ASSIGNEE(S): Cell Pathways, Inc., USA  
SOURCE: U.S., 19 pp.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6060477	A	20000509	US 1995-484002	19950607
US 6391885	B1	20020521	US 2000-564196	20000504
PRIORITY APPLN. INFO.:			US 1995-484002	A3 19950607
OTHER SOURCE(S):		MARPAT 132:321870		

GI



I

AB A method for treating precancerous lesions comprises administration of  
title compds. [I; R1-R3 = H, halo, alkyl, alkoxy, alkenyl, alkenyloxy,

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alkylthio, alkylamino, cyano, acylamino, etc.; R4 = H, alkyl, alkoxy, Ph, OH, halo, acylamino, aminoacyl, 5-tetrazolyl, cyano, etc.; X1-X4 = N, C;  $\geq 1$  of X1-X4 = N,  $\geq 1$  of X1-X4 = C] (no data). Thus, 2-propoxybenzoyl chloride in MeCN was added to a mixture of 2-aminonicotinamide and Et3N in MeCN at 0° followed by 1.5 h stirring and standing overnight to give 2-(2-propoxybenzamido)nicotinamide. This was refluxed 30 min. with pyridine in aqueous NaOH to give 2-(2-propoxyphenyl)pyrido[2,3-d]pyrimid-4(3H)-one. A capsule formulation containing the latter is given.

IT 127979-73-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of pyridopyrimidinones, pyrimidopyrimidinones, pyrimidotriazinones, and related compds. for the treatment of precancerous lesions)

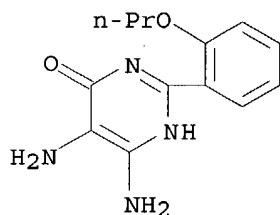
RN 127979-73-1 CAPLUS

CN 4(1H)-Pyrimidinone, 5,6-diamino-2-(2-propoxyphenyl)-, sulfate (1:1) (9CI)  
(CA INDEX NAME)

CM 1

CRN 57075-34-0

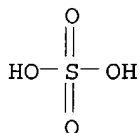
CMF C13 H16 N4 O2



CM 2

CRN 7664-93-9

CMF H2 O4 S



REFERENCE COUNT: 126 THERE ARE 126 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 14 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:511159 CAPLUS

DOCUMENT NUMBER: 131:157709

TITLE: Preparation of bicyclic pyridine and pyrimidine derivatives as neuropeptide Y receptor antagonists  
INVENTOR(S): Norman, Mark H.; Chen, Ning; Han, Nianhe; Liu, Longbin; Hurt, Clarence R.; Fotsch, Christopher H.; Jenkins, Tracy J.; Moreno, Ofir A.

PATENT ASSIGNEE(S): Amgen Inc., USA

SOURCE: PCT Int. Appl., 469 pp.

CODEN: PIXXD2

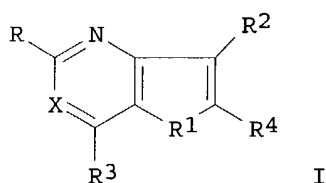


09/ 811,359

DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9940091	A1	19990812	WO 1999-US2500	19990205
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
US 6187777	B1	20010213	US 1999-246775	19990204
CA 2319275	AA	19990812	CA 1999-2319275	19990205
AU 9926590	A1	19990823	AU 1999-26590	19990205
AU 747920	B2	20020530		
EP 1054887	A1	20001129	EP 1999-906756	19990205
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2003502272	T2	20030121	JP 2000-530520	19990205
ZA 9900967	A	19990806	ZA 1999-967	19990208
US 6583154	B1	20030624	US 2000-640263	20000816
PRIORITY APPLN. INFO.:				
			US 1998-73927P	P 19980206
			US 1998-73981P	P 19980206
			US 1998-93482P	P 19980720
			US 1998-93577P	P 19980720
			US 1999-246775	A 19990204
			WO 1999-US2500	W 19990205

OTHER SOURCE(S): MARPAT 131:157709  
GI



AB Title compds.[I; R = H, CH<sub>3</sub>, (CH<sub>3</sub>)<sub>2</sub>CH, SCH<sub>3</sub>, CH<sub>3</sub>CH<sub>2</sub>, NH<sub>2</sub>, CF<sub>3</sub>, NHCOC<sub>6</sub>H<sub>5</sub>, cyclopropyl, CH<sub>2</sub>OH, (CH<sub>3</sub>)<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>, N(CH<sub>3</sub>)<sub>2</sub>, OCH<sub>3</sub>, NHCH<sub>3</sub>, NH(CH<sub>2</sub>)<sub>4</sub>NH<sub>2</sub>; R<sub>1</sub> = NH, S, NCH<sub>3</sub>, O; R<sub>2</sub> = H, COCH<sub>3</sub>, C<sub>6</sub>H<sub>5</sub>, CH<sub>3</sub>, CH<sub>3</sub>CH<sub>2</sub>; R<sub>3</sub> = NH<sub>2</sub>, CH<sub>3</sub>, NHC<sub>6</sub>H<sub>5</sub>, N(CH<sub>2</sub>CH<sub>3</sub>)<sub>2</sub>, (CH<sub>3</sub>CH<sub>2</sub>)N(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>, (CH<sub>3</sub>)N(CH<sub>2</sub>)<sub>2</sub>NHCH<sub>3</sub>, N(CH<sub>3</sub>)CH(CH<sub>3</sub>)CH(Ph)OH, (CH<sub>3</sub>CH<sub>2</sub>)NCH<sub>2</sub>C(CH<sub>3</sub>):CH<sub>2</sub>, NHCH<sub>2</sub>CF<sub>3</sub>, NHCH<sub>2</sub>CH<sub>2</sub>C<sub>6</sub>H<sub>5</sub>, NH(CH<sub>2</sub>)<sub>3</sub>OCH<sub>2</sub>CH<sub>3</sub>, 4-ClC<sub>6</sub>H<sub>4</sub>, 4-CH<sub>3</sub>OC<sub>6</sub>H<sub>5</sub>, 2-thienyl, 1-pyrrolidinyl, 1-piperidinyl, 4-morpholinyl, 1-piperazinyl, 3-pyridyl; R<sub>4</sub> = C<sub>6</sub>H<sub>5</sub>, 4-CH<sub>3</sub>C<sub>6</sub>H<sub>4</sub>, 4-ClC<sub>6</sub>H<sub>4</sub>, (CH<sub>3</sub>)<sub>3</sub>C, 4-FC<sub>6</sub>H<sub>4</sub>, 3-HOC<sub>6</sub>H<sub>4</sub>, 2-pyridyl, cyclohexyl, 2-furyl, 2-FC<sub>6</sub>H<sub>4</sub> 2-thienyl, 1-adamantyl, CH<sub>3</sub>, 4-CH<sub>3</sub>OC<sub>6</sub>H<sub>4</sub>; X = N, CH; etc.], pharmaceutical acceptable salts, ester, solvate, and N-oxide are prepared and tested as neuropeptide Y receptor antagonists in the modulation of feeding behavior, obesity, diabetes, cancer, inflammatory disorders, depression, stress related disorders, Alzheimer's disease and other disease conditions. Thus, the title compound I (R = CH<sub>3</sub>; R<sub>1</sub> = NH; X = N; R<sub>2</sub> = H; R<sub>3</sub> = N(CH<sub>2</sub>CH<sub>3</sub>)<sub>2</sub>; R<sub>4</sub> = C<sub>6</sub>H<sub>5</sub>) was prepared

IT 237435-23-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT

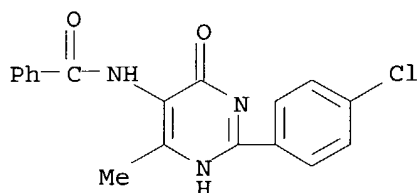
09/ 811,359

(Reactant or reagent)

(preparation of pyrrolopyridine and pyrrolopyrimidine derivs. as  
neuropeptide Y receptor antagonists)

RN 237435-23-3 CAPLUS

CN Benzamide, N-[2-(4-chlorophenyl)-1,4-dihydro-6-methyl-4-oxo-5-pyrimidinyl]-  
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS  
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 15 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:375547 CAPLUS

DOCUMENT NUMBER: 131:31952

TITLE: Preparation of 2-aryl-8-oxodihydropurine derivatives  
as anxiolytics

INVENTOR(S): Murata, Teruya; Masumoto, Kaoru; Kondo, Katsunori;  
Furukawa, Kiyoshi; Oka, Makoto

PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 86 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

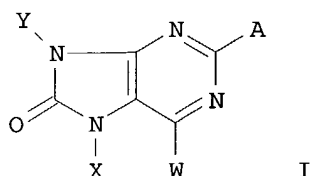
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9928320	A1	19990610	WO 1998-JP5320	19981126
W:	AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
ZA 9810490	A	19990520	ZA 1998-10490	19981117
TW 502034	B	20020911	TW 1998-87119571	19981125
CA 2312885	AA	19990610	CA 1998-2312885	19981126
AU 9912604	A1	19990616	AU 1999-12604	19981126
AU 744014	B2	20020214		
EP 1036794	A1	20000920	EP 1998-955937	19981126
EP 1036794	B1	20030827		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO			
BR 9815140	A	20001010	BR 1998-15140	19981126
NZ 504457	A	20011221	NZ 1998-504457	19981126
AT 248169	E	20030915	AT 1998-955937	19981126
RU 2223272	C2	20040210	RU 2000-117278	19981126
US 6372740	B1	20020416	US 2000-555490	20000601
NO 2000002835	A	20000724	NO 2000-2835	20000602
PRIORITY APPLN. INFO.:			JP 1997-350000	A 19971203
			WO 1998-JP5320	W 19981126

09/ 811,359

GI



AB Title compds. I (W = H, alkyl, halo, alkoxy, amino, alkylamino, Ph, substituted Ph; X = H, alkyl, alkenyl, carbamoyl, etc.; Y = H, alkyl, cycloalkyl, alkenyl, etc.; A = Ph, substituted Ph, heteroaryl, etc.) and their pharmaceutically acceptable salts, useful as anxiolytics (no data), were prepared. Thus, reaction of 7,9-dihydro-9-methyl-2-phenyl-8H-purin-8-one with 2-bromo-N-ethyl-N-phenyl-acetamide in DMF in the presence of NaH at room temperature for 3 h gave N-ethyl-8,9-dihydro-9-methyl-8-oxo-2-phenyl-N-phenyl-7H-purine-7-acetamide. Formulations containing I were given.

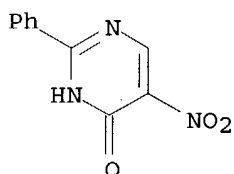
IT 3749-46-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 2-aryl-8-oxodihydropurine derivs. as anxiolytics)

RN 3749-46-0 CAPLUS

CN 4(1H)-Pyrimidinone, 5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L10 ANSWER 16 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:314282 CAPLUS

DOCUMENT NUMBER: 129:54385

TITLE: Preparation of acetic acid amide derivatives as drugs

INVENTOR(S): Murata, Akiya; Hino, Katsuhiko; Furukawa, Kiyoshi; Oka, Makoto; Ito, Mari

PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 44 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

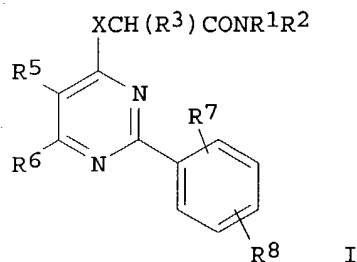
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10130150	A2	19980519	JP 1997-257573	19970905
PRIORITY APPLN. INFO.:			JP 1996-257704	19960905
OTHER SOURCE(S):		MARPAT 129:54385		

GI



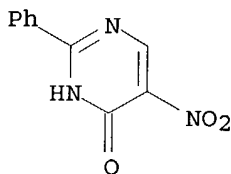
AB The title compds. [I; X = O, NR<sub>4</sub>; R<sub>1</sub> = H, (un)substituted lower alkyl or alkenyl, etc.; R<sub>2</sub> = cycloalkyl, lower alkyl, (un)substituted Ph, etc.; R<sub>3</sub> = H, alkyl, hydroxyalkyl, etc.; R<sub>4</sub> = H, alkyl, or combine with R<sub>3</sub> and N to form a pyrrolidine or piperidine; R<sub>5</sub> = H, lower alkyl or alkenyl, hydroxyalkyl, CF<sub>3</sub>, etc.; R<sub>6</sub> = H, lower alkyl, CF<sub>3</sub>, etc.; R<sub>7</sub> = H, halo, lower alkyl, etc.; R<sub>8</sub> = H, halo, lower alkoxy, etc.] are prepared I, possessing affinity toward the benzodiazepine receptor, are useful for prevention and treatment of melancholia, insecure related diseases, central nervous system diseases, and immunity inflammation diseases. Thus, 4-chloro-5,6-dimethyl-2-phenylpyrimidine was reacted with 2-amino-N,N-dipropylacetamide in the presence of Et<sub>3</sub>N to give I (R<sub>1</sub> = R<sub>2</sub> = n-Pr, R<sub>3</sub> = R<sub>7</sub> = R<sub>8</sub> = H, R<sub>5</sub> = R<sub>6</sub> = Me, X = NH), which showed IC<sub>50</sub> of 3.10 nM with abenzodiazepine receptor (BZ<sub>03</sub>) when tested with rat. A formulation containing I was also prepared

IT 3749-46-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of acetic acid amide derivs. as drugs)

RN 3749-46-0 CAPLUS

CN 4(1H)-Pyrimidinone, 5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 17 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:407610 CAPLUS

DOCUMENT NUMBER: 127:121691

TITLE: Synthesis of 4,6-disubstituted and 4,5,6-trisubstituted 2-phenylpyrimidines and their affinity towards A1 adenosine receptors

AUTHOR(S): Biagi, Giuliana; Giorgi, Irene; Livi, Oreste; Scartoni, Valerio; Lucacchini, Antonio

CORPORATE SOURCE: Dip. Scienze Farmaceutiche, Univ. Pisa, Pisa, 56126, Italy

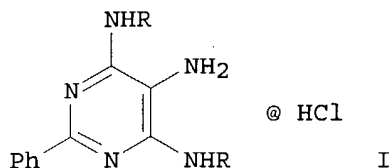
SOURCE: Farmaco (1997), 52(1), 61-65  
CODEN: FRMCE8; ISSN: 0014-827X

PUBLISHER: Societa Chimica Italiana

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB The preparation and assay of the title compds., e.g., I (R = cyclohexyl, pentyl), are reported. The results support our hypothesis about the possibility that mols. characterized by great flexibility, such as 2-phenyl-4,5,6-triaminopyrimidines, can better interact with the receptor sites than rigid mols. such as 2,6,9-trisubstituted 8-azaadenines. The relatively low activity shown by pyrimidine derivs. demonstrated the importance of the bicyclic aromatic system in 8-azaadenines and adenines for a favorable interaction with the A1 adenosine receptors.

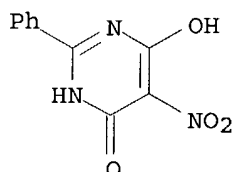
IT 68905-99-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 4,6-disubstituted and 4,5,6-trisubstituted 2-phenylpyrimidines and their A1 adenosine receptor affinity)

RN 68905-99-7 CAPLUS

CN 4(1H)-Pyrimidinone, 6-hydroxy-5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 18 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:753799 CAPLUS

DOCUMENT NUMBER: 126:18884

TITLE: Preparation and formulation of pyrimidine derivatives as agents with effect on the peripheral benzodiazepine receptors

INVENTOR(S): Murata, Teruya; Hino, Katsuhiko; Furukawa, Kiyoshi; Oka, Makoto; Itoh, Mari

PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 110 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9632383	A1	19961017	WO 1996-JP977	19960410
W:	AL, AM, AT, AU, AZ, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KR, KZ, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK			
RW:	KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML			
IL 117659	A1	20001206	IL 1996-117659	19960326
ZA 9602438	A	19961001	ZA 1996-2438	19960327

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CA 2218033	AA	19961017	CA 1996-2218033	19960410
AU 9652874	A1	19961030	AU 1996-52874	19960410
AU 694647	B2	19980723		
EP 826673	A1	19980304	EP 1996-909327	19960410
EP 826673	B1	20021120		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI				
CN 1186487	A	19980701	CN 1996-194408	19960410
CN 1094929	B	20021127		
BR 9604894	A	19980714	BR 1996-4894	19960410
RU 2160256	C2	20001210	RU 1997-118591	19960410
SK 281840	B6	20010806	SK 1997-1374	19960410
CZ 289093	B6	20011017	CZ 1997-3223	19960410
RO 117532	B1	20020430	RO 1997-1858	19960410
AT 228113	E	20021215	AT 1996-909327	19960410
PT 826673	T	20030228	PT 1996-96909327	19960410
ES 2187644	T3	20030616	ES 1996-909327	19960410
TW 450963	B	20010821	TW 1996-85104372	19960412
NO 9704685	A	19971212	NO 1997-4685	19971010
US 5972946	A	19991026	US 1997-930604	19971014

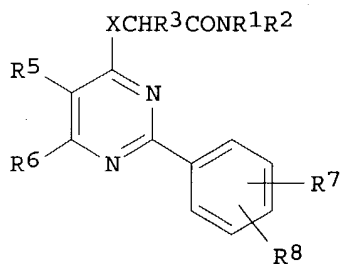
PRIORITY APPLN. INFO.:

JP 1995-113937 A 19950413  
WO 1996-JP977 W 19960410

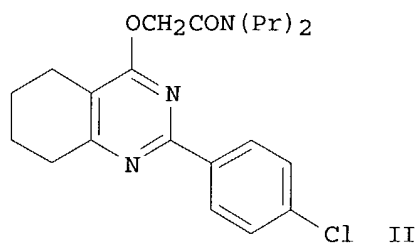
OTHER SOURCE(S):

MARPAT 126:18884

GI



I



II

AB The title compds. I [X represents O or NR<sub>4</sub>; R<sub>1</sub> represents H, lower alkyl, lower alkenyl or cycloalkyl(lower)alkyl; R<sub>2</sub> represents lower alkyl, cycloalkyl, optionally substituted Ph, etc.; R<sub>3</sub> represents H, lower alkyl or hydroxy(lower)alkyl; R<sub>4</sub> represents H, lower alkyl, etc.; R<sub>5</sub> represents hydroxy(lower)alkyl, etc.; R<sub>6</sub> represents H, lower alkyl, CF<sub>3</sub> or optionally substituted Ph, or R<sub>5</sub> and R<sub>6</sub> together form (CH<sub>2</sub>)<sub>n</sub>; n = 3 - 6; R<sub>7</sub> represents H, halogeno, lower alkyl, lower alkoxy, CF<sub>3</sub>, OH, NH<sub>2</sub>, etc.; and R<sub>8</sub> represents H, halogeno, lower alkyl or lower alkoxy] are prepared. In an in vitro test for affinity for the peripheral benzodiazepine receptors, the title compound II in vitro showed IC<sub>50</sub> of 0.89 nM.

IT 3749-46-0P

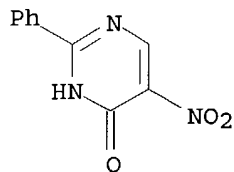
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of pyrimidine derivs. as agents with effect on peripheral benzodiazepine receptors)

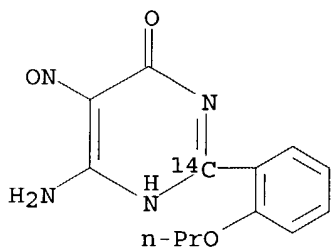
RN 3749-46-0 CAPLUS

CN 4(1H)-Pyrimidinone, 5-nitro-2-phenyl- (9CI) (CA INDEX NAME)

09/ 811,359



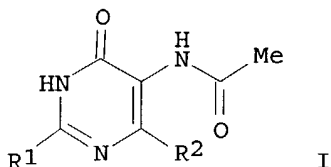
L10 ANSWER 19 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1995:777454 CAPLUS  
DOCUMENT NUMBER: 123:340001  
TITLE: Carbon-14 labeled nitrogen heterocycles. The syntheses of these phosphodiesterase inhibitors  
AUTHOR(S): Lawrie, Kenneth W. M.; Novelli, Christine E. A.; Saunders, David; Coastes, William J.  
CORPORATE SOURCE: New Frontiers Sci. Park, SmithKline Beecham Pharm. Res. Dev. Synth. Isotope Chem. Dep., Essex, CM19 5AW, UK  
SOURCE: Journal of Labelled Compounds & Radiopharmaceuticals (1995), 36(9), 891-8  
CODEN: JLCRD4; ISSN: 0362-4803  
PUBLISHER: Wiley  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB The syntheses of three heterocyclic phosphodiesterase inhibitors are described from a common radiolabeled precursor, namely 2-propoxybenzo[cyano-14C]nitrile. Conversion of the nitrile to the corresponding Me ketone or amidine allows elaboration of the heterocycles radiolabeled within the ring systems. The target compds. were [14C]-labeled 7-(cyclopropylamino)-2-(2-propoxyphenyl)pyrimido[4,5-d]pyrimidin-4(1H)-one (SF&K 97992) and 1,7-dihydro-2-(2-propoxyphenyl)-6H-purin-6-one (SF&K 96231).  
IT 170703-44-3P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation of [14C]-labeled purinone and pyrimido[4,5-d]pyrimidinone)  
RN 170703-44-3 CAPLUS  
CN 4(1H)-Pyrimidinone-2-14C, 6-amino-5-nitroso-2-(2-propoxyphenyl)- (9CI)  
(CA INDEX NAME)



L10 ANSWER 20 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1995:691725 CAPLUS  
DOCUMENT NUMBER: 123:111733  
TITLE: Synthesis of 2,6-disubstituted 5-aminopyrimidine-4-ones from 2,6-disubstituted 5-acetylpyrimidin-4-one oximes through Beckmann rearrangement  
AUTHOR(S): Yamamoto, Yutaka; Ogawa, Yoshitaka  
CORPORATE SOURCE: Tohoku Coll. Pharm., Komatsushima 4-chome, Sendai,

09/ 811,359

SOURCE: 981, Japan  
Yakugaku Zasshi (1995), 115(3), 256-60  
CODEN: YKKZAJ; ISSN: 0031-6903  
PUBLISHER: Pharmaceutical Society of Japan  
DOCUMENT TYPE: Journal  
LANGUAGE: Japanese  
OTHER SOURCE(S): CASREACT 123:111733  
GI

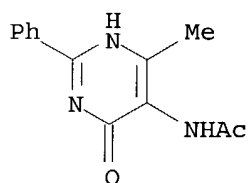


AB 2,6-Disubstituted 5-acetylpyrimidin-4-one oximes were heated in formic acid under reflux to undergo Beckmann rearrangement, giving 2,6-disubstituted 5-acetylaminopyrimidin-4-ones (I; R1, R2 = Ph, Me; p-ClC6H4, Me; Ph, p-MeC6H4; Ph, 3-pyridyl) in good yields.

IT 72168-63-9P  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(synthesis of disubstituted 5-aminopyrimidineones from disubstituted 5-acetylpyrimidinone oximes through Beckmann rearrangement)

RN 72168-63-9 CAPLUS

CN Acetamide, N-(1,4-dihydro-6-methyl-4-oxo-2-phenyl-5-pyrimidinyl)- (9CI)  
(CA INDEX NAME)



L10 ANSWER 21 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:655817 CAPLUS

DOCUMENT NUMBER: 121:255817

TITLE: Process for preparation of cycloalkyl- and azacycloalkylpyrrolopyrimidines useful as GABA<sub>A</sub> receptor ligands

INVENTOR(S): Thurkauf, Andrew; Hutchison, Alan; Singh, Vinod

PATENT ASSIGNEE(S): Neurogen Corp., USA

SOURCE: Braz. Pedido PI, 101 pp.  
CODEN: BPXXDX

DOCUMENT TYPE: Patent

LANGUAGE: Portuguese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
BR 9201262	A	19931013	BR 1992-1262	19920408
RU 2055077	C1	19960227	RU 1992-5011467	19920406
RO 109942	B1	19950728	RO 1992-478	19920407



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PRIORITY APPLN. INFO.:

SU 1992-5011467 A 19920406

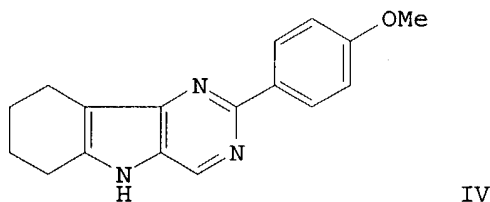
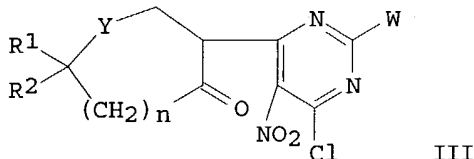
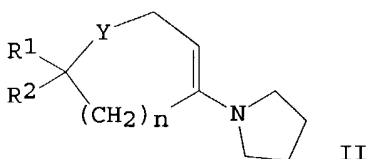
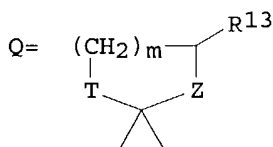
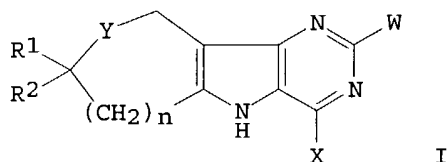
BR 1992-1262

19920408

OTHER SOURCE(S):

MARPAT 121:255817

GI



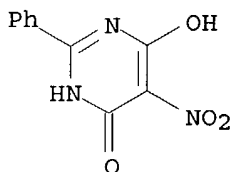
AB Title compds. I [ $n = 0, 1, 2$ ;  $R_1, R_2 = H, \text{alkyl}$ ;  $X = H, OH$ ;  $W =$  (un)substituted Ph, thienyl, pyridyl;  $Y = NR_3, CO, CR_6(OR_5), CR_6(COR_5), CR_6(CO_2R_5), CR_6(OCOR_5), CR_5R_6, CR_6(CONR_7R_8), CR_6[(CH_2)_nNR_7R_8], CR_6(NR_9CO_2R_{10}), CR_6[C(OH)R_{11}R_{12}]$ , cyclic group Q;  $R_3 = H, \text{alkyl, Ph, pyridyl, phenylalkyl, (di)(alkyl)aminoalkyl, (un)substituted 1-indanyl, 4-(thio)chromanyl, or 1,2,3,4-tetrahydro-1-naphthyl, COR_4, SO_2R_4$ ;  $R_4 = \text{alkyl, Ph, phenylalkyl, phenylalkoxy}$ ;  $R_5, R_8, R_9, R_{10}, R_{13}, R_{14} = H, \text{alkyl, Ph, pyridyl, phenylalkyl}$ ;  $R_6, R_7 = H, \text{alkyl}$ ; or  $NR_7R_8 = \text{morpholino, piperidino, pyrrolidino, or N-alkylpiperazino}$ ;  $R_{11}, R_{12} = \text{alkyl, Ph, phenylalkyl}$ ;  $m = 0, 1, 2$ ;  $Z = CH_2, O, NR_{14}, CHCONR_{14}$  (sic);  $T = CH_2, O$ ] were prepared (77 examples). I are highly selective agonists, antagonists, inverse agonists, or prodrugs for cerebral GABA<sub>A</sub> receptors, and are useful for diagnosis or treatment of anxiety, convulsions, sleep disturbances, or benzodiazepine overdose, or for improving activity (sic). Preparation of I involves 5 steps: (1) reaction of dialkyl malonates with arylamidines  $WC(:NH)NH_2$  to give 2-aryl-4,6-dihydroxypyrimidines; (2) nitration of these in the 5-position; (3) treatment of the resultant arylnitrodihydroxypyrimidines with  $POCl_3$  to give 2-aryl-5-nitro-4,6-dichloropyrimidines; (4) coupling of these with cyclic pyrrolidine enamines II to give 4-substituted 5-nitro-6-chloropyrimidines III; and (5) catalytic hydrogenation of III with cyclization. In tests for binding to rat cortical GABA<sub>A</sub> receptors in vitro, 12 selected I had  $IC_{50}$  of 0.009-1.00  $\mu M$ , e.g., 0.039  $\mu M$  for IV, a preferred compound

IT 68905-99-7P, 4(1H)-Pyrimidinone, 6-hydroxy-5-nitro-2-phenyl-  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of GABAergic cycloalkyl- and azacycloalkylpyrrolopyrimidines)

RN 68905-99-7 CAPLUS

CN 4(1H)-Pyrimidinone, 6-hydroxy-5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 22 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1994:655782 CAPLUS  
 DOCUMENT NUMBER: 121:255782  
 TITLE: Preparation of aryl heterocyclyl pyrimidines as GABA brain receptor ligands  
 INVENTOR(S): Thurkauf, Andrew; Hutchison, Alan  
 PATENT ASSIGNEE(S): Neurogen Corp., USA  
 SOURCE: U.S., 17 pp. Cont. of U.S. Ser. No. 865,129, abandoned.  
 CODEN: USXXAM  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5326868	A	19940705	US 1993-106193	19930812
WO 9425463	A1	19941110	WO 1993-US3917	19930430
W: AT, AU, BB, BG, BR, BY, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, RO, RU, SD, SE, SK, UA, US, UZ, VN				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9341174	A1	19941121	AU 1993-41174	19930430
US 5463054	A	19951031	US 1994-269667	19940701
PRIORITY APPLN. INFO.:			US 1992-865129	19920408
			WO 1993-US3917	19930430
			US 1993-106193	19930812

OTHER SOURCE(S): MARPAT 121:255782

GI For diagram(s), see printed CA Issue.

AB Title compds. I (X = H, halo, HO; W = (substituted) aryl; A, B, C, D, E = C or N substituted with H or various organic and inorg. substituents; R3, R4 = organic and inorg. substituents), are prepared 2-(2-Fluoro-4-methoxyphenyl)6,7,8,9-tetrahydro-5H-indolo[3,2-d]pyrimidine and Pd black in mesitylene was stirred at 230° to give the title compound 2-(2-fluoro-4-methoxyphenyl)5H-indolo[3,2-d]pyrimidine. I demonstrated GABAA receptor activity.

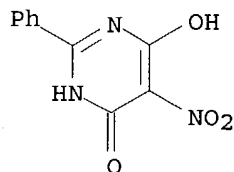
IT **68905-99-7P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of aryl heterocyclyl pyrimidines as GABA brain receptor ligands)

RN 68905-99-7 CAPLUS

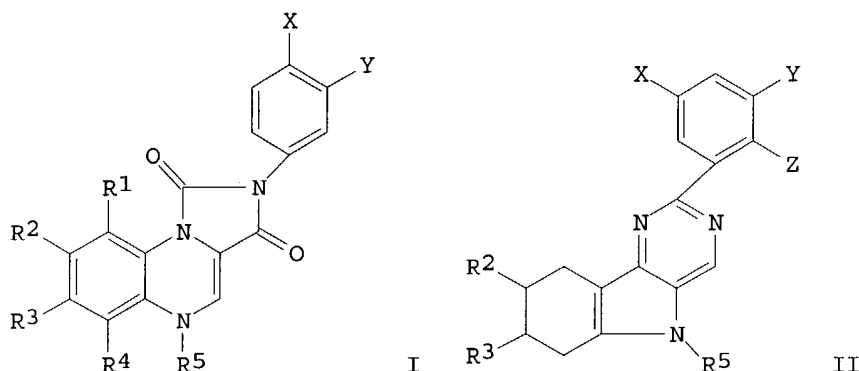
CN 4(1H)-Pyrimidinone, 6-hydroxy-5-nitro-2-phenyl- (9CI) (CA INDEX NAME)

09/ 811,359



L10 ANSWER 23 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1994:95809 CAPLUS  
DOCUMENT NUMBER: 120:95809  
TITLE: Novel GABAA receptor subtypes and methods for  
screening drug compounds using imidazoquinoxalines and  
pyrrolopyrimidines to bind to GABAA receptor subtypes  
INVENTOR(S): Shaw, Kenneth; Hutchison, Alan; Thurkauf, Andrew;  
Tallman, John  
PATENT ASSIGNEE(S): Neurogen Corp., USA  
SOURCE: PCT Int. Appl., 36 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9322681	A1	19931111	WO 1993-US3920	19930430
W:	AT, AU, BB, BG, BR, CA, CH, CZ, DE, DK, ES, FI, GB, HU, JP, KP, KR, KZ, LK, LU, MG, MN, MW, NL, NO, NZ, PL, RO, RU, SD, SE, SK, UA, US, VN			
RW:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
US 5597920	A	19970128	US 1992-876050	19920430
AU 9341177	A1	19931129	AU 1993-41177	19930430
AU 691470	B2	19980521		
EP 639275	A1	19950222	EP 1993-910819	19930430
EP 639275	B1	19970917		
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE			
JP 08500333	T2	19960116	JP 1993-519445	19930430
AT 158414	E	19971015	AT 1993-910819	19930430
ES 2110090	T3	19980201	ES 1993-910819	19930430
US 5688654	A	19971118	US 1994-331501	19941028
PRIORITY APPLN. INFO.:			US 1992-876050	19920430
			WO 1993-US3920	19930430
OTHER SOURCE(S):	MARPAT 120:95809			
GI				



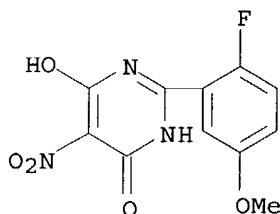
AB Imidazoquinoxalines I and pyrrolopyrimidines II (R1-R4, X, Y = H, halo, alkyl, alkoxy; R5 = H, lower alkyl; Z = H, F) bind selectively to a novel subtype of the GABA<sub>A</sub> binding site. Selective interaction of ligands at this unique receptor population results in pharmacol. specificity which may lead to superior anxiolytics, cognition enhancers, anticonvulsants, and hypnotics. Such drugs may be screened by measuring their competition with 3H- or I isotope-labeled I or II for binding to these GABA<sub>A</sub> receptors. Thus, I (R1-R5, Y = H; X = OEt) (III) bound with high affinity (K<sub>i</sub> 0.5 nM) to rat cortical GABA<sub>A</sub> receptors. III-3H was prepared by reaction of 2-nitrophenyl isocyanate, 3-bromo-4-ethoxyaniline, and ClCH<sub>2</sub>COCl, reduction of the NO<sub>2</sub> group with Fe powder to cyclize, further bromination in positions 6 and 8, and tritiation with T<sub>2</sub> over Pd/C.

IT 152336-01-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and chlorination of)

RN 152336-01-1 CAPLUS

CN 4(1H)-Pyrimidinone, 2-(2-fluoro-5-methoxyphenyl)-6-hydroxy-5-nitro- (9CI)  
(CA INDEX NAME)



L10 ANSWER 24 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:582837 CAPLUS

DOCUMENT NUMBER: 119:182837

TITLE: Arylazopyrimidines as dichroic dyes for liquid crystals

AUTHOR(S): Mikhaleva, M. A.; Igonina, G. A.; Lazareva, V. T.; Romyantsev, V. G.; Mamaev, V. P.

CORPORATE SOURCE: Novosib. Inst. Org. Khim., Novosibirsk, 630090, Russia  
SOURCE: Khimiya Geterotsiklicheskih Soedinenii (1993), (2), 209-14

CODEN: KGSSAQ; ISSN: 0132-6244

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB Substituted 5- and 2-(arylazo)pyrimidines were synthesized and studied for

09/ 811,359

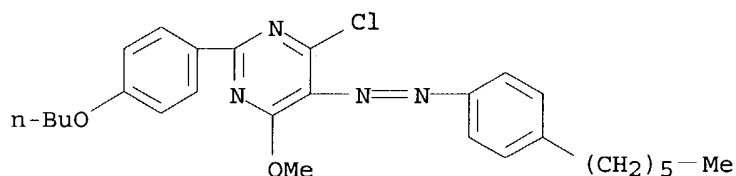
potential application as dichroic dyes with pos. dichroism for color liquid-crystal. optical imaging devices. Absorption spectra ( $\lambda_{\max}$  = 368-474 nm) and order parameters ( $S$  = 0.38-0.71) were determined for 8 dyes. A dye with optimum properties ( $S$  = 0.71,  $\lambda_{\max}$  = 474 nm) is prepared by 2-[4-(hexyloxy)phenyl]-5-aminopyrimidine condensation with 1-(dimethylamino)-4-nitrosobenzene in superbasic medium.

IT 150563-33-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and characterization of, as potential dichroic dye for color liquid-crystal. optical imaging devices)

RN 150563-33-0 CAPLUS

CN Pyrimidine, 2-(4-butoxyphenyl)-4-chloro-5-[(4-hexylphenyl)azo]-6-methoxy-(9CI) (CA INDEX NAME)



L10 ANSWER 25 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:448538 CAPLUS

DOCUMENT NUMBER: 117:48538

TITLE: Preparation of 6,7,8,9-tetrahydro-5H-indolo[3.2-d]pyrimidines and analogs as GABA receptor ligands

INVENTOR(S): Thurkauf, Andrew; Hutchison, Alan; Singh, Vinod

PATENT ASSIGNEE(S): Neurogen Corp., USA

SOURCE: PCT Int. Appl., 75 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

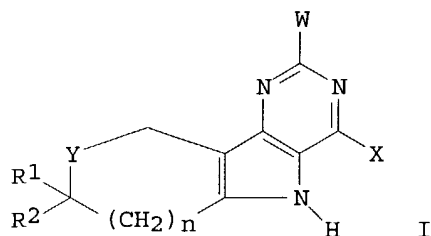
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9206094	A1	19920416	WO 1991-US7195	19911008
W: AU, CA, JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE				
CA 2091986	AA	19920410	CA 1991-2091986	19911008
CA 2091986	C	19951128		
AU 9187326	A1	19920428	AU 1991-87326	19911008
AU 652968	B2	19940915		
EP 552237	A1	19930728	EP 1991-918267	19911008
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 06502147	T2	19940310	JP 1991-517025	19911008
EP 738717	A1	19961023	EP 1996-105337	19911008
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 5216159	A	19930601	US 1991-800885	19911127
CZ 281084	B6	19960612	CZ 1992-779	19920316
CN 1076929	A	19931006	CN 1992-102339	19920331
IN 175034	A	19950422	IN 1992-CA218	19920401
US 5585490	A	19961217	US 1993-30468	19930405

PRIORITY APPLN. INFO.: US 1990-594712 A2 19901009  
EP 1991-918267 A3 19911008  
WO 1991-US7195 A 19911008

OTHER SOURCE(S): MARPAT 117:48538

GI



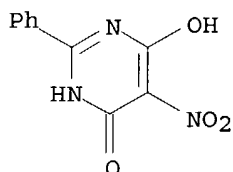
AB Title compds. I [ $n = 0-2$ ;  $R_1, R_2 = H$ , C1-6 alkyl;  $X = H$ , OH;  $W =$  (substituted) Ph, -thienyl, -pyridyl;  $Y = NR_3$ , CO, CR6OR5, CR6COR5, CR6CO2R5, CR6OCOR5R6, etc.;  $R_3 = H$ , C1-6 alkyl, Ph, pyridyl, phenyl-C1-6 alkyl, aminoalkyl, 1-indanyl, etc.;  $R_5 = H$ , C1-6 alkyl, Ph, pyridyl, phenyl-C1-6 alkyl;  $R_6 = H$ , C1-6 alkyl] and related compds. were prepared as GABA receptor ligands. Thus, the enamine formed from cyclohexanone and pyrrolidine was arylated by treatment with 2-phenyl-5-nitro-4,6-dichloropyrimidine (preparation given) and  $(Me_2CH)_2EtN$  in  $CH_2Cl_2$  and the product formed was hydrogenated in EtOH containing  $Et_3N$  and 10% Pd/C to give 2-phenyl-6,7,8,9-tetrahydro-5H-indolo[3,2-d]-pyrimidine (II). II had  $IC_{50}$  of 0.100  $\mu M$  against 3H-flumazenil binding to GABA receptors.

IT **68905-99-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as intermediate for GABA receptor ligands)

RN 68905-99-7 CAPLUS

CN 4(1H)-Pyrimidinone, 6-hydroxy-5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 26 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:164270 CAPLUS

DOCUMENT NUMBER: 114:164270

TITLE: Preparation of phenylpyrimidone derivatives as inhibitors of a calmodulin-insensitive cyclic GMP phosphodiesterase

INVENTOR(S): Coates, William John

PATENT ASSIGNEE(S): Smith Kline and French Laboratories Ltd., UK

SOURCE: Eur. Pat. Appl., 12 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 400799	A1	19901205	EP 1990-304313	19900423
EP 400799	B1	19940112		
R: CH, DE, FR, GB, IT, LI, NL				
JP 02295977	A2	19901206	JP 1990-109945	19900424
US 5290933	A	19940301	US 1991-794311	19911114
PRIORITY APPLN. INFO.:			GB 1989-9558	19890426

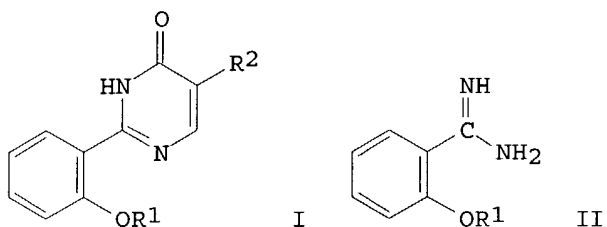
09/ 811,359

US 1990-514385

19900425

OTHER SOURCE(S):  
GI

MARPAT 114:164270



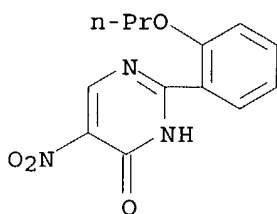
AB The title compds. (I; R1 = alkyl, alkenyl, cycloalkylalkyl, phenylalkyl, fluoroalkyl; R2 = H, NH2, alkanoylamino, CONR3R4; R4 = alkyl; R5 = H, alkyl), useful as vasodilators and antihypertensives and for treatment of asthma, bronchitis, and congestive heart failure, are prepared by cyclocondensation of benzamidines (II) with XCH:CR6CO2R7 (X = leaving group; R6 = any group R2 or its precursor; R7 = an ester forming group). Thus, cyclocondensation of II (R1 = Pr) with EtOCH:C(NO2)CO2Et in EtOH containing EtONa followed by acidification with aqueous HCl gave I (R2 = NO2) which was hydrogenated over 10 % Pd/C in MeOH to give I (R2 = NH2). I (R2 = AcNH) (II) at 3.8  $\mu$ mol/kg reduced the U46619-induced bronchoconstriction by 50% in guinea-pigs. Soft gelatin capsules containing II were formulated.

IT 133152-11-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and acidification of)

RN 133152-11-1 CAPLUS

CN 4(1H)-Pyrimidinone, 5-nitro-2-(2-propoxyphenyl)-, sodium salt (9CI) (CA  
INDEX NAME)



● Na

L10 ANSWER 27 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:499389 CAPLUS

DOCUMENT NUMBER: 113:99389

TITLE: Metal-complex azo dyes for textile, leather and metal applications

INVENTOR(S): Puentener, Alois; Burdeska, Kurt

PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.

SOURCE: Eur. Pat. Appl., 21 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

09/ 811,359

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 357554	A2	19900307	EP 1989-810623	19890822
EP 357554	A3	19900912		
R: BE, CH, DE, ES, FR, GB, LI				
US 4962191	A	19901009	US 1989-399202	19890828
JP 02117962	A2	19900502	JP 1989-226384	19890831
PRIORITY APPLN. INFO.:			CH 1988-3238	19880831
OTHER SOURCE(S):	MARPAT 113:99389			
GI				

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title dyes I [D1, D2 = (un)substituted diazobenzene or naphthalene component having a OH or CO2H group ortho to the azo group; D3 = (un)substituted coupling benzene, naphthalene, or heterocyclic residue in which X is ortho to the azo group; M = Cr, Co; Q = (un)substituted Ph, naphthyl, or aromatic heterocyclic residue; R1 = (un)substituted C1-6 alkyl or Ph; R2 = H, R1; X = O, NR3; R3 = H, C1-4 alkyl; p, q = 0, 1], useful for dyeing rayon, natural cellulose fibers, protein fibers, polyimide fibers, polyurethane fibers, basic-modified polyolefin fibers, leather, pelts, or anodized Al, are prepared Thus, 3-amino-4-hydroxy-5-nitrobenzenesulfonic acid was diazotized and coupled with 4-(ethylamino)-6-hydroxy-2-phenylpyrimidine, and the azo intermediate complexed with Co sulfate, producing the 1:2 chrome-complex dye II, which dyed leather a fast red shade.

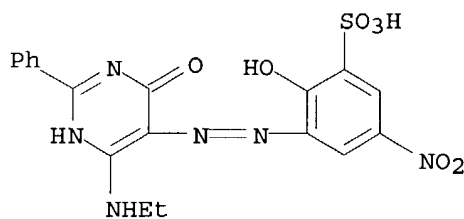
IT 129010-15-7P

RL: PREP (Preparation)

(manufacture of, as intermediate for metal complex azo dyes)

RN 129010-15-7 CAPLUS

CN Benzenesulfonic acid, 3-[[6-(ethylamino)-1,4-dihydro-4-oxo-2-phenyl-5-pyrimidinyl]azo]-2-hydroxy-5-nitro- (9CI) (CA INDEX NAME)



L10 ANSWER 28 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:440713 CAPLUS

DOCUMENT NUMBER: 113:40713

TITLE: Alkoxyphenylpurines as inhibitors of calmodulin-insensitive cyclic GMP phosphodiesterase

INVENTOR(S): Coates, William John

PATENT ASSIGNEE(S): Smith Kline and French Laboratories Ltd., UK

SOURCE: Eur. Pat. Appl., 17 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

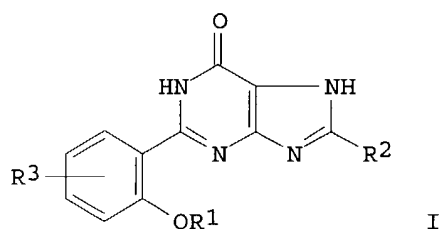
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:



PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 352960	A2	19900131	EP 1989-307341	19890719
EP 352960	A3	19911106		
EP 352960	B1	19941026		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AU 8938210	A1	19900125	AU 1989-38210	19890718
AU 613503	B2	19910801		
US 5073559	A	19911217	US 1989-382610	19890719
DK 8903636	A	19900126	DK 1989-3636	19890721
ZA 8905613	A	19900530	ZA 1989-5613	19890724
JP 02088577	A2	19900328	JP 1989-192462	19890725
PRIORITY APPLN. INFO.:			GB 1988-17651	19880725
OTHER SOURCE(S):	MARPAT 113:40713			
GI				



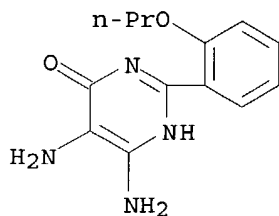
AB The title compds. [I; R1 = (fluoro)alkyl, alkenyl, cycloalkylalkyl, phenylalkyl; R2 = H, OH, alkyl, Ph, SH, alkylthio, CF3, amino; R3 = H, NO2, amino, alkanoylamino, alkoxy, alkyl, halo, SO2NR4R5, CONR4R5, alkylthio, alkylsulfonyl, CN, etc.; R4, R5 = H, alkyl] were prepared as inhibitors of calmodulin-insensitive cyclic GMP phosphodiesterase. Thus, 2-(2-propoxy-5-chlorophenyl)purin-6-one (II) was prepared in 6 steps from 5-chloro-2-hydroxybenzamide via 2-(5-chloro-2-propoxyphenyl)-4-amino-5-nitrosopyrimidin-6-one. II at 16.6  $\mu\text{mol/kg}$  i.v. in guinea pigs gave 30% inhibition of ovalbumin-induced bronchoconstriction. A capsule formulation containing II is given.

IT 57075-34-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclocondensation of, with acetamide hydrochloride)

RN 57075-34-0 CAPLUS

CN 4(1H)-Pyrimidinone, 5,6-diamino-2-(2-propoxyphenyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 29 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:423942 CAPLUS

DOCUMENT NUMBER: 113:23942

TITLE: Preparation of condensed pyrimidine derivatives as inhibitors of calmodulin insensitive cyclic GMP

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phosphodiesterase  
INVENTOR(S): Coates, William John; Rawlings, Derek Anthony  
PATENT ASSIGNEE(S): Smith Kline and French Laboratories Ltd., UK  
SOURCE: Eur. Pat. Appl., 19 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 349239	A2	19900103	EP 1989-306453	19890626
EP 349239	A3	19900718		
EP 349239	B1	19940316		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 5075310	A	19911224	US 1989-370494	19890623
AT 102945	E	19940415	AT 1989-306453	19890626
AU 8937099	A1	19900104	AU 1989-37099	19890627
AU 614389	B2	19910829		
DK 8903228	A	19900102	DK 1989-3228	19890628
ZA 8904942	A	19910626	ZA 1989-4942	19890629
JP 02056484	A2	19900226	JP 1989-171017	19890630
PRIORITY APPLN. INFO.:			GB 1988-15716	19880701
			GB 1988-15717	19880701
			GB 1988-15718	19880701
			EP 1989-306453	19890626

OTHER SOURCE(S): MARPAT 113:23942

GI For diagram(s), see printed CA Issue.

AB The title compds. (I; ring A = Q-Q2; X = O, S; R1 = C1-6 alkyl, C2-6 alkenyl, C3-5 cycloalkyl, C1-4 alkyl, C1-4 alkyl substituted by 1-6 F), useful for treatment of asthma and bronchitis and also as vasodilators in treatment of angina, hypertension, and congestive heart failure, are prepared by (1) cyclocondensation of 2-R1OC6H4R2 [II; R2 = C(:NH)NH2] with a pyrazole derivative (III; R3 = C1-4 alkoxy, NH2) to give I (ring A = Q), (2) cyclization of II (R2 = Q3) to give I (ring A = Q, Q1), (3) oxidative cyclization of II (R2 = Q4, X1 = nitroso) to give I (ring A = Q2, X = O), and (4) cyclocondensation of II (R2 = Q4, X1 = NH2) with SOCl2 to give I (ring A = Q2, X = S). Thus, a mixture of II [R1 = Pr, R2 = C(:NH)NH2].MeSO3H, II (R3 = NH2).H2SO4, and AcONa was heated 1 h in an oil bath (180°) to give I (R1 = Pr, ring A = Q). Also prepared were I (R1 = Pr; ring A = Q1, Q2 where X = O, S). Three I at 2.62-5.13 µmol/kg inhibited 50% the bronchoconstriction induced by U46619 (9,11-methanoepoxy-PGH2) in guinea pigs.

IT 119409-17-5

RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclocondensation of, with thionyl chloride)

RN 119409-17-5 CAPLUS

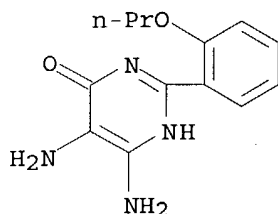
CN 4(1H)-Pyrimidinone, 5,6-diamino-2-(2-propoxyphenyl)-, sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 57075-34-0

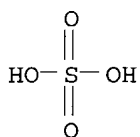
CMF C13 H16 N4 O2

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CM 2

CRN 7664-93-9  
CMF H2 O4 S



L10 ANSWER 30 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1990:406363 CAPLUS  
DOCUMENT NUMBER: 113:6363  
TITLE: Fused pyrimidine derivatives, process and intermediates for their preparation and pharmaceutical compositions containing them  
INVENTOR(S): Coates, William John; Flynn, Seyn Thomas; Rawlings, Derek Anthony  
PATENT ASSIGNEE(S): Smith Kline and French Laboratories Ltd., UK  
SOURCE: Eur. Pat. Appl., 29 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 347146	A2	19891220	EP 1989-305911	19890612
EP 347146	A3	19900711		
EP 347146	B1	19930901		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
AT 93858	E	19930915	AT 1989-305911	19890612
ES 2058527	T3	19941101	ES 1989-305911	19890612
US 5047404	A	19910910	US 1989-365469	19890613
AU 8936357	A1	19891221	AU 1989-36357	19890614
AU 612852	B2	19910718		
DK 8902970	A	19891217	DK 1989-2970	19890615
ZA 8904563	A	19910130	ZA 1989-4563	19890615
JP 02042079	A2	19900213	JP 1989-155560	19890616
JP 2815617	B2	19981027		
PRIORITY APPLN. INFO.:				
			GB 1988-14350	A 19880616
			GB 1988-14351	A 19880616
			GB 1988-14353	A 19880616
			EP 1989-305911	A 19890612
OTHER SOURCE(S): MARPAT 113:6363				
GI For diagram(s), see printed CA Issue.				

09/ 811,359

AB Title compds. I [R1 = (substituted C1-6 alkyl, C2-6 alkenyl, C3-5 cycloalkyl-C1-6 alkyl; R2 = C1-6 alkylthio, C1-6 alkylsulfonyl, C1-6 alkoxy, HO, H, H2NNH, C1-6 alkyl, Ph, R3CONH, R3 = H, C1-6 alkyl, R4R5N = pyrrolidino, piperidino, morpholino, etc.; A = pyrido, (substituted) pyrazino, triazino] are prepared as bronchodilators, antiallergics, vasodilators, and inhibitors of a calmodulin insensitive cyclic GMP phosphodiesterase. 2-PrOC6H4COCl in MeCN was added dropwise to 2-aminonicotinamide and Et3N in MeCN to give 2-(2-propoxybenzamido)nicotinamide which with pyridine in 2N NaOH was refluxed for 30 min to give II, which was effective in controlling allergic reactions at 28 µmol/kg i.v. in guinea pigs. Also prepared were 22 addnl. I which showed bronchodilation, vasodilation, antiallergy activity and phosphodiesterase inhibition. A capsule formulation comprising II was given.

IT 127488-22-6

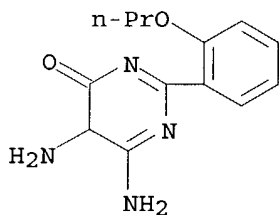
RL: RCT (Reactant); RACT (Reactant or reagent)  
(reaction of, in preparation of fused pyrimidine pharmaceuticals)

RN 127488-22-6 CAPLUS

CN 4(5H)-Pyrimidinone, 5,6-diamino-2-(2-propoxyphenyl)-, sulfate (1:1) (9CI)  
(CA INDEX NAME)

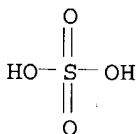
CM 1

CRN 127488-21-5  
CMF C13 H16 N4 O2



CM 2

CRN 7664-93-9  
CMF H2 O4 S



L10 ANSWER 31 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:114815 CAPLUS

DOCUMENT NUMBER: 110:114815

TITLE: Preparation and formulation of 2-(2-alkoxyphenyl)-6-purinone derivatives as pharmaceuticals

PATENT ASSIGNEE(S): Smith Kline and French Laboratories Ltd., UK

SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

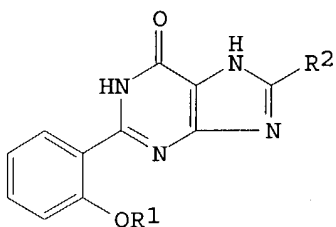
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PATENT INFORMATION:

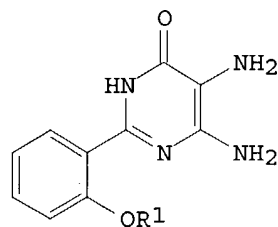
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63196585	A2	19880815	JP 1988-23631	19880201
CA 1303037	A1	19920609	CA 1988-557327	19880126
DK 8800407	A	19880803	DK 1988-407	19880127
EP 293063	A1	19881130	EP 1988-300696	19880127
EP 293063	B1	19920318		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
US 4885301	A	19891205	US 1988-148791	19880127
AT 73802	E	19920415	AT 1988-300696	19880127
ES 2033423	T3	19930316	ES 1988-300696	19880127
AU 8810956	A1	19880804	AU 1988-10956	19880129
AU 599452	B2	19900719		
ZA 8800680	A	19880928	ZA 1988-680	19880201
PRIORITY APPLN. INFO.:			GB 1987-2300	19870202
			GB 1987-2301	19870202
			EP 1988-300696	19880127

OTHER SOURCE(S): MARPAT 110:114815

GI



I



II

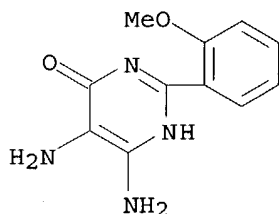
AB The title compds. (I; R1 = C1-6 alkyl, C2-6 alkenyl; R2 = H, OH), useful as bronchodilators and vasodilators, are prepared A mixture of 1.5 g diaminopyrimidinone salt II.H2SO4 (R1 = Pr) and HCONH2 was heated 70 min at 190-200° to give 0.72 g purinone I (R1 = Pr, R2 = H) (III), which had an ED50 of 3.6 µmol/kg against bronchoconstriction in guinea pigs and an IC50 of 0.96 µM for inhibition of phosphodiesterase extracted from pig arteries. Soft gelatin capsules were prepared each containing III 3.0, soy bean oil 88.2, and hydrogenated vegetable shortening-beeswax 8.8 weight%.

IT 57075-32-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclocondensation of, with amides)

RN 57075-32-8 CAPLUS

CN 4(1H)-Pyrimidinone, 5,6-diamino-2-(2-methoxyphenyl)- (9CI) (CA INDEX NAME)

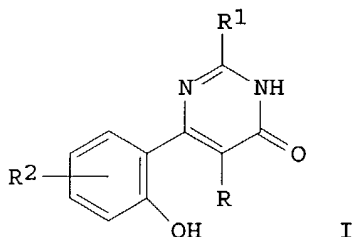


09/ 811,359

DOCUMENT NUMBER: 109:211073  
TITLE: Preparation and testing of 5-amino-6-(2-hydroxyphenyl)pyrimidin-4(3H)-one derivatives as analgesics  
INVENTOR(S): Tanaka, Masaaki; Ogura, Kuniyoshi; Morita, Hikari; Aozuka, Tomoshi; Nakada, Naoki; Takagi, Kaname  
PATENT ASSIGNEE(S): Zeria Pharmaceutical Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63030473	A2	19880209	JP 1986-173555	19860725
PRIORITY APPLN. INFO.:			JP 1986-173555	19860725
OTHER SOURCE(S):	MARPAT	109:211073		

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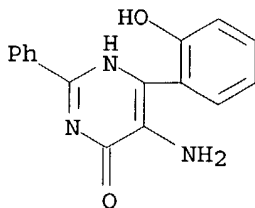
AB The title compds. [I; R = NH<sub>2</sub>, R<sub>1</sub> = lower alkyl, (un)substituted Ph, NH<sub>2</sub>, cyclic amino; R<sub>2</sub> = H, lower alkyl, lower alkoxy, halo] (II) were prepared as analgesics. MeC(:NH)NH<sub>2</sub>·HCl was added to a solution of Na in EtOH and the mixture was stirred at room temperature for 10 min. To the mixture, 4-methoxy-3-nitrocoumarin was added and the mixture was refluxed for 1 h to give 70% I (R = NO<sub>2</sub>, R<sub>1</sub> = Me, R<sub>2</sub> = H) which was hydrogenated over 5% Pd/C in EtOH to give 50% I (R = NH<sub>2</sub>, R<sub>1</sub> = Me, R<sub>2</sub> = H) (IV). IV at 30 mg/kg p.o. exhibited 68.3% inhibition of AcOH-induced writhing in mice whereas aminopyrine showed 38.9% inhibition.

IT 110566-03-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of, as analgesic)

RN 110566-03-5 CAPLUS

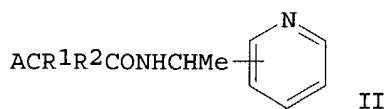
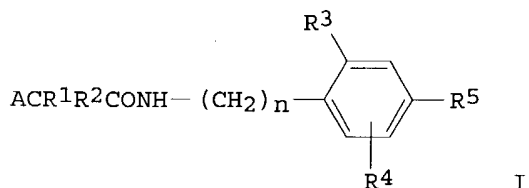
CN 4(1H)-Pyrimidinone, 5-amino-6-(2-hydroxyphenyl)-2-phenyl- (9CI) (CA INDEX NAME)



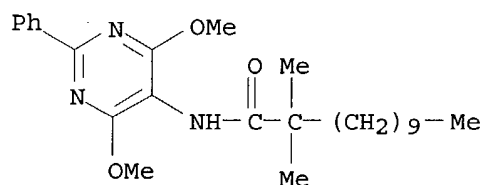
09/ 811,359

L10 ANSWER 33 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1988:417030 CAPLUS  
DOCUMENT NUMBER: 109:17030  
TITLE: Saturated fatty acid amides as inhibitors of  
acyl-CoA:cholesterol acyltransferase  
INVENTOR(S): Hoefle, Milton L.; Holmes, Ann; Roth, Bruce D.  
PATENT ASSIGNEE(S): Warner-Lambert Co., USA  
SOURCE: U.S.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4716175	A	19871229	US 1987-17960	19870224
US 4743605	A	19880510	US 1987-103316	19871001
CA 1336913	A1	19950905	CA 1988-557467	19880127
ZA 8800604	A	19890927	ZA 1988-604	19880128
AU 8811354	A1	19880825	AU 1988-11354	19880205
AU 610558	B2	19910523		
FI 8800796	A	19880825	FI 1988-796	19880219
FI 89593	B	19930715		
FI 89593	C	19931025		
DK 8800941	A	19880825	DK 1988-941	19880223
DK 165406	B	19921123		
DK 165406	C	19930413		
NO 8800774	A	19880825	NO 1988-774	19880223
NO 174043	B	19931129		
NO 174043	C	19940309		
EP 283742	A2	19880928	EP 1988-102644	19880223
EP 283742	A3	19890726		
EP 283742	B1	19930526		
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE				
JP 63253060	A2	19881020	JP 1988-38777	19880223
JP 07121895	B4	19951225		
AT 89814	E	19930615	AT 1988-102644	19880223
ES 2056843	T3	19941016	ES 1988-102644	19880223
US 4716175	B1	19930622	US 1990-90002032	19900529
PRIORITY APPLN. INFO.:			US 1987-17960	19870224
			EP 1988-102644	19880223
OTHER SOURCE(S):		CASREACT 109:17030		
GI				



- AB Title phenylalkyl amides I and pyridylalkyl amides II (A = C1-20 hydrocarbyl containing 1-3 double bonds; R1 = H, C1-4 alkyl, PhCH2; R2 = C1-4 alkyl, PhCH2; CR1R2 = saturated C3-7 carbocyclic ring; R3-R5 = H, F, Cl, Br, CF3, C1-4 alkyl, C1-4 alkoxy, n = 0, 1) are prepared, and are useful for inhibiting intestinal absorption of cholesterol. MeCH(CO2Et)2 was treated with NaOEt, and alkylated with 1-bromotetradecane, followed by hydrolysis to give 2-methyl-2-tetradecylmalonic acid, which was thermally decarboxylated to form 2-methylhexadecanoic acid. The latter compound was transformed into the acid chloride and treated with 2,4,6-trimethoxyphenylamine-HCl to form N-(2,4,6-trimethoxyphenyl)-2-methylhexadecanamide. 2,2-Dimethyl-N-(2,4,6-trimethoxyphenyl)dodecanamide (50 mg/kg) was administered orally 30 min prior to each meal to cholesterol-loaded rabbits fed a high cholesterol diet; after 7 days, there was a 67% decrease in serum cholesterol, compared to cholesterol-loaded nontreated controls.
- IT **114289-67-7P**  
 RL: SPN (Synthetic preparation); PREP (Preparation)  
 (preparation of, for inhibition of absorption of dietary cholesterol)
- RN 114289-67-7 CAPLUS
- CN Dodecanamide, N-(4,6-dimethoxy-2-phenyl-5-pyrimidinyl)-2,2-dimethyl- (9CI)  
 (CA INDEX NAME)



L10 ANSWER 34 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1987:547168 CAPLUS

DOCUMENT NUMBER: 107:147168

TITLE: Synthesis and analgesic activity of  
 4-amino-1,2-dihydro-5-(2-hydroxyphenyl)-3H-pyrazol-3-ones and 5-amino-6-(2-hydroxyphenyl)pyrimidin-4(3H)-ones

AUTHOR(S): Takagi, Kaname; Tanaka, Masaaki; Morita, Hikari;  
 Ogura, Kuniyoshi; Ishii, Katsuyuki; Nakata, Naoki;  
 Ozeki, Masayuki

CORPORATE SOURCE: Cent. Res. Lab., Zeria Pharm. Co., Saitama, 360-01, Japan

SOURCE: European Journal of Medicinal Chemistry (1987), 22(3), 239-42  
 CODEN: EJMCA5; ISSN: 0223-5234

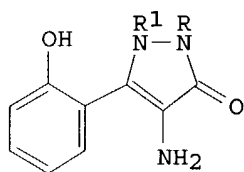
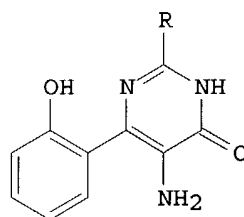
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 107:147168

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I, R=R<sup>1</sup>=HII, R=Me, R<sup>1</sup>=HIII, R=H, R<sup>1</sup>=Me

IV, R=Me

V, R=C<sub>6</sub>H<sub>4</sub>NH<sub>2</sub>-4

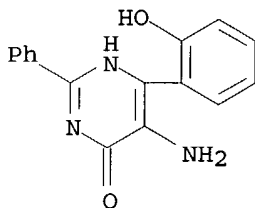
AB Three 4-amino-1,2-dihydro-5-(2-hydroxyphenyl)-3-H-pyrazol-3-ones and six 5-amino-6-(2-hydroxyphenyl)pyrimidin-4(3H)-ones were synthesized from 4-methoxy- and 4-hydroxy-3-nitrocoumarins, and tested for analgesic activity upon oral administration to mice. Most of the compds. prepared exhibited analgesic activity which was superior to that of aminopyrine. In particular, the pyrazolones I, II, and III and the pyrimidinones IV and V, showed prominent activity, which was 3-4.5 times as potent as that of aminopyrine.

IT 110566-03-5P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation and analgesic activity of)

RN 110566-03-5 CAPLUS

CN 4(1H)-Pyrimidinone, 5-amino-6-(2-hydroxyphenyl)-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 35 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1986:129853 CAPLUS

DOCUMENT NUMBER: 104:129853

TITLE: Synthesis of 2-substituted 4-oxo-5-nitropyrimidines from methyl 3-ethoxy-2-nitroacrylate and other reactions

AUTHOR(S): De la Cuesta, E.; Avendano, C.

CORPORATE SOURCE: Fac. Farm., Univ. Complutense, Madrid, Spain

SOURCE: Journal of Heterocyclic Chemistry (1985), 22(2), 337-9

CODEN: JHTCAD; ISSN: 0022-152X

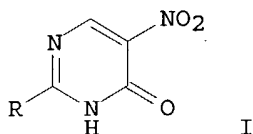
DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 104:129853

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AB Nitropyrimidines I (R = NH<sub>2</sub>, Me, Ph) were prepared by cyclization of EtOCH:C(NO<sub>2</sub>)CO<sub>2</sub>Me (II) and HN:CR(NH<sub>2</sub>). Condensation of II with H<sub>2</sub>NNHCOR<sub>1</sub> (R<sub>1</sub> = Me, Ph) yielded R<sub>1</sub>CONHNHCH:C(NO<sub>2</sub>)CO<sub>2</sub>Me which could not be cyclized.

IT 99893-00-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and neutralization of, with acetic acid)

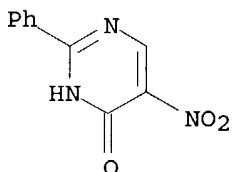
RN 99893-00-2 CAPLUS

CN Benzenecarboximidamide, compd. with 5-nitro-2-phenyl-4(1H)-pyrimidinone (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 3749-46-0

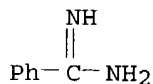
CMF C10 H7 N3 O3



CM 2

CRN 618-39-3

CMF C7 H8 N2



L10 ANSWER 36 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:406360 CAPLUS

DOCUMENT NUMBER: 103:6360

TITLE: N-(2-Nitrophenyl)-5-aminopyrimidine derivatives and their use

INVENTOR(S): Zondler, Helmut; Hubele, Adolf; Nyfeler, Robert

PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.

SOURCE: Eur. Pat. Appl., 92 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

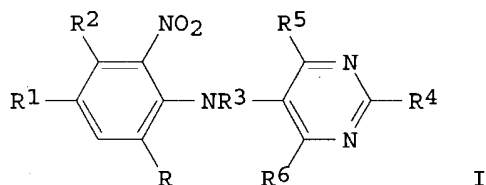
FAMILY ACC. NUM. COUNT: 1

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PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 132826	A1	19850213	EP 1984-108700	19840723
EP 132826	B1	19880928		
R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE				
US 4840662	A	19890620	US 1984-631272	19840716
IL 72478	A1	19871220	IL 1984-72478	19840720
CA 1218370	A1	19870224	CA 1984-459440	19840723
AT 37540	E	19881015	AT 1984-108700	19840723
DK 8403620	A	19850126	DK 1984-3620	19840724
AU 8430998	A1	19850214	AU 1984-30998	19840724
AU 577053	B2	19880915		
ZA 8405703	A	19850327	ZA 1984-5703	19840724
BR 8403677	A	19850702	BR 1984-3677	19840724
ES 534577	A1	19850716	ES 1984-534577	19840724
JP 60051178	A2	19850322	JP 1984-155129	19840725
PRIORITY APPLN. INFO.:			CH 1983-4047	19830725
			EP 1984-108700	19840723

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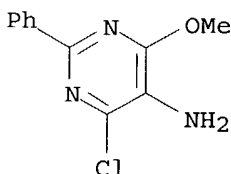
AB Seventy-four title compds. I [R, R1 = H, NO2, CF3; R2 = H, halo; R3 = H, COR7 [R7 = (un)substituted alkyl]; R4 = H, halo, NO2, cyano, SH, thiocyanato, alkyl, haloalkyl, substituted cycloalkoxy, alkenyloxy, alkynyloxy, alkylthio, alkenylthio, alkylsulfonyl, alkylsulfinyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl, dialkylamino, (un)substituted alkoxy, Ph, PhCH2; R5, R6 = H, halo, NO2, cyano, SH, thiocyanato, alkyl, haloalkyl, (un)substituted alkoxy, substituted cycloalkoxy, alkenyloxy, alkynyloxy, alkylthio, alkenylthio, alkylsulfonyl, alkylsulfinyl, alkenyl, alkenylthio, alkylsulfonyl, alkylsulfinyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl, dialkylamino] were prepared Thus, 2.84 g 5-amino-4-chloro-6-methoxypyrimidine in 20 mL DMSO at 15° was treated dropwise with 6.24 g 1,3-dichloro-2,6-dinitro-4-(trifluoromethyl)benzene and 2.30 g KOCMe3 in 15 mL DMSO to give 2.52 g I (R = NO2, R1 = CF3, R2 = R5 = Cl, R3 = R4 = H, R6 = OMe), which at 0.02% inhibited Puccinia graminis on wheat by 95-100%.

IT 96833-44-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
(amination by, of chlorobenzene derivative)

RN 96833-44-2 CAPLUS

CN 5-Pyrimidinamine, 4-chloro-6-methoxy-2-phenyl- (9CI) (CA INDEX NAME)



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L10 ANSWER 37 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1985:150903 CAPLUS  
DOCUMENT NUMBER: 102:150903  
TITLE: Fluorescent dyes for solar collectors  
AUTHOR(S): Iden, Ruediger; Seybold, Guenther; Stange, Andreas;  
Eilingsfeld, Heinz  
CORPORATE SOURCE: ZD/Farbenlab., BASF A.-G., Ludwigshafen, Fed. Rep.  
Ger.  
SOURCE: Forschungsber. - Bundesminist. Forsch. Technol.,  
Technol. Forsch. Entwickl. (1984), BMFT-FB-T 84-164,  
115 pp.  
CODEN: BFTEAJ; ISSN: 0340-7608  
DOCUMENT TYPE: Report  
LANGUAGE: German

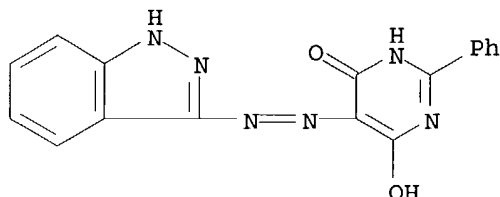
AB A large number of organic dyes was synthesized and screened for potential use in solar collectors. Most suitable were perylene and perylene imide dyes, B complexes of naphtholactam dyes, and polycarbocyclic dyes. These compds. covered the whole color range from yellow to blue. Chromatog. methods were developed for purification of fluorescent dyes.

IT 95689-94-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclization of)

RN 95689-94-4 CAPLUS

CN 4(1H)-Pyrimidinone, 6-hydroxy-5-(1H-indazol-3-ylazo)-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 38 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1984:591957 CAPLUS  
DOCUMENT NUMBER: 101:191957  
TITLE: 2-Aryl-4,6-dihalopyrimidines as antidotes for  
protecting cultivated plants from damage by herbicides  
INVENTOR(S): Brunner, Hans Georg  
PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.  
SOURCE: Eur. Pat. Appl., 42 pp.  
CODEN: EPXXDW

DOCUMENT TYPE: Patent  
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 3

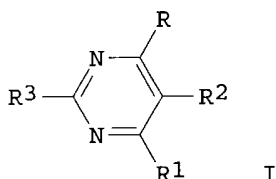
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 112280	A2	19840627	EP 1983-810514	19831109
EP 112280	A3	19850925		
EP 112280	B1	19900829		
R: BE, CH, DE, FR, GB, IT, LI, NL				
US 4648896	A	19870310	US 1983-549038	19831107
CA 1233819	A1	19880308	CA 1983-440899	19831110
BR 8306261	A	19840619	BR 1983-6261	19831114
ZA 8308467	A	19840627	ZA 1983-8467	19831114

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ES 527234	A1	19851116	ES 1983-527234	19831114
IL 70231	A1	19890630	IL 1983-70231	19831114
JP 59104365	A2	19840616	JP 1983-214945	19831115
PRIORITY APPLN. INFO.:			CH 1982-6650	19821115
			IL 1981-64612	19811221

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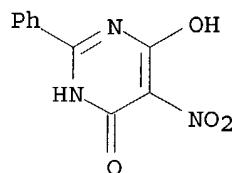
AB The title compds. [I; R, R1 = halo; R2 = amino, acyl, thiocyanato, R4Z (R4 = H, acyl, alkynyl, (un)substituted alkyl, alkenyl; Z = O, S, SO, SO2), R3 = (un)substituted Ph, thienyl, furyl] were prepared Thus, 2-phenyl-4,6-pyrimidinediol was nitrated to give I (R = R1 = OH, R2 = NO2, R3 = Ph). This was chlorinated by POCl3 in the presence of PhNMe2 and hydrogenated over Raney Ni to give I (R = R1 = Cl, R2 = NH2, R3 = Ph) (II). At 100 ppm II gave 50% protection to rice seedlings treated with the herbicide pretilachlor at 0.25 kg/ha.

IT 68905-99-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and chlorination of)

RN 68905-99-7 CAPLUS

CN 4(1H)-Pyrimidinone, 6-hydroxy-5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 39 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1982:406048 CAPLUS

DOCUMENT NUMBER: 97:6048

TITLE: A one-step synthesis of purine derivatives by the reaction of phenylazomalonamidamine with aryl aldehydes

AUTHOR(S): Yoneda, Fumio; Koga, Ryosuke; Higuchi, Masatsugu

CORPORATE SOURCE: Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, 862, Japan

SOURCE: Chemistry Letters (1982), (3), 365-8

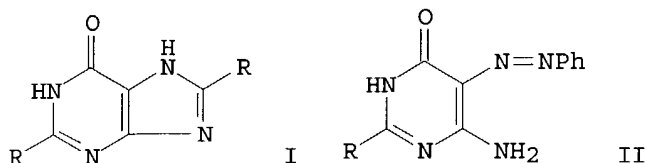
CODEN: CMLTAG; ISSN: 0366-7022

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 97:6048

GI



AB Treatment of  $\text{H}_2\text{NCOCH}(\text{N}:\text{NPh})\text{C}(:\text{NH})\text{NH}_2\cdot\text{HCl}$  with  $\text{RCHO}$  ( $\text{R} = \text{Ph}$ , substituted  $\text{Ph}$ ) yielded the 2,8-diarylhydropyrimidines I in a single step. Under milder conditions the reaction formed  $\text{H}_2\text{NCOCH}(\text{N}:\text{NPh})\text{C}(:\text{NH})\text{N}:\text{CHR}\cdot\text{HCl}$ , from which the phenylazopyrimidine-4(3H)-ones II were obtained by oxidative cyclization with  $\text{EtO}_2\text{CN}:\text{NCO}_2\text{Et}$ . Treatment of II with a second aryl aldehyde gave the unsym. 2,8-diarylated hypoxanthines.

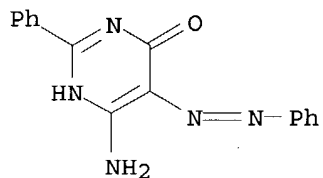
IT **54014-72-1P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with aromatic aldehydes)

RN 54014-72-1 CAPLUS

CN 4(1H)-Pyrimidinone, 6-amino-2-phenyl-5-(phenylazo)- (9CI) (CA INDEX NAME)



L10 ANSWER 40 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1980:639357 CAPLUS

DOCUMENT NUMBER: 93:239357

TITLE: Use of the Vilsmeier reaction in the synthesis of pyrrolo [3,2-d]pyrimidine-7-aldehyde derivatives

AUTHOR(S): Sizova, O. S.; Britikova, N. E.; Novitskii, K. Yu.; Shcherbakova, L. I.; Pershin, G. N.

CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR

SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1980), 14(7), 63-6

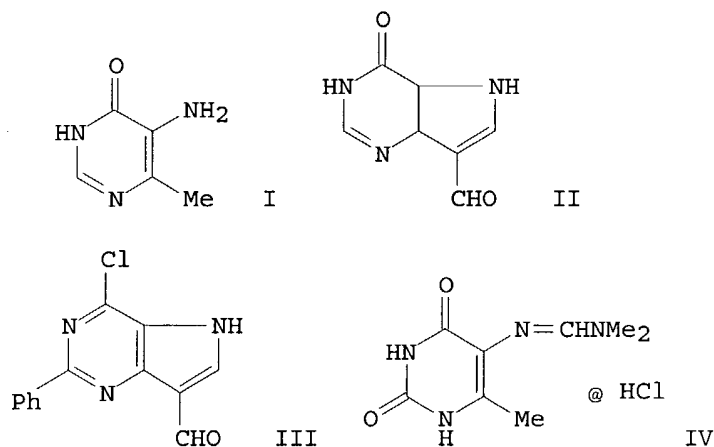
CODEN: KHFZAN; ISSN: 0023-1134

DOCUMENT TYPE: Journal

LANGUAGE: Russian

OTHER SOURCE(S): CASREACT 93:239357

GI



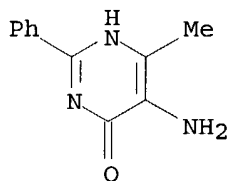
AB Vilsmeier reaction of pyrimidinone I, prepare from thiourea and MeCOCH(NHAc)CO<sub>2</sub>Et via a pyrimidinethione, gave 70% aldehyde II. Aldehyde III was prepared similarly. Formamidine IV was prepared by Vilsmeier reaction of 5-amino-6-methyluracil. The phenylhydrazones of III suppressed the growth of lactic acid bacteria.

IT 72168-62-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
(Vilsmeier reaction of)

RN 72168-62-8 CAPLUS

CN 4(1H)-Pyrimidinone, 5-amino-6-methyl-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 41 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1980:604635 CAPLUS

DOCUMENT NUMBER: 93:204635

TITLE: Penicillins and their salts

INVENTOR(S): Wetzell, Bernd; Woitun, Eberhard; Reuter, Wolfgang;

Maier, Roland; Lechner, Uwe; Goeth, Hanns

PATENT ASSIGNEE(S): Thomae, Dr. Karl, G.m.b.H., Fed. Rep. Ger.

SOURCE: Ger. Offen., 53 pp. Addn. to Ger. Offen. 2,808,153.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

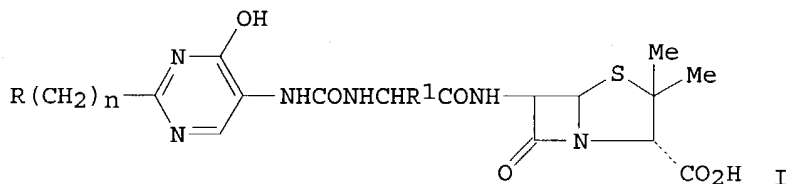
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2851270	A1	19800612	DE 1978-2851270	19781127
ES 477520	A1	19790601	ES 1979-477520	19790207
EP 3814	A2	19790905	EP 1979-100468	19790219
EP 3814	A3	19791017		
EP 3814	B1	19811216		

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R: BE, CH, DE, FR, GB, IT, LU, NL, SE

AT 7901282	A	19810315	AT 1979-1282	19790220
AT 364459	B	19811027		
US 4241056	A	19801223	US 1979-13006	19790221
DK 7900774	A	19790826	DK 1979-774	19790222
FI 7900614	A	19790826	FI 1979-614	19790223
FI 68237	B	19850430		
FI 68237	C	19850812		
NO 7900628	A	19790828	NO 1979-628	19790223
AU 7944559	A1	19790920	AU 1979-44559	19790223
AU 522042	B2	19820513		
IL 56731	A1	19820430	IL 1979-56731	19790223
HU 23633	O	19820928	HU 1979-T01096	19790223
HU 180997	B	19830530		
JP 54122291	A2	19790921	JP 1979-21790	19790226
JP 60058237	B4	19851219		
CA 1132539	A1	19820928	CA 1979-322301	19790226
AT 8003862	A	19810415	AT 1980-3862	19800725
US 31926	E	19850625	US 1982-420804	19820921
PRIORITY APPLN. INFO.:			DE 1978-2808153	19780225
			DE 1978-2851226	19781127
			DE 1978-2851270	19781127
			US 1979-13006	19790221

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AB The penicillins I (R = optionally substituted Ph; R1 = Ph, 4-HOC6H4, 1,4-cyclohexadienyl; n = 0, 1) were prepared Thus 4-ClC6H4CH2C(:NH)NH2 was condensed with EtO2CNHC(:CHONa)CO2Et to give 42.5% 5-amino-2-p-chlorobenzyl-4-pyrimidinol which was treated with COCl2 and amoxycillin-3H2O to give 73% I (R = 4-ClC6H4, R1 = 4-HOC6H4, n = 1) as the Na salt.

IT **75424-41-8**

RL: RCT (Reactant); RACT (Reactant or reagent)  
(acylation of aminopenicillanic acid by)

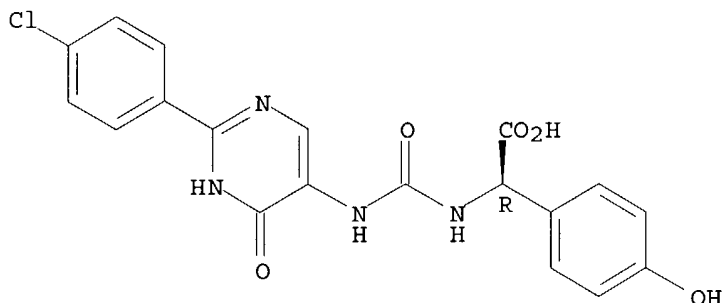
RN 75424-41-8 CAPLUS

CN Benzeneacetic acid,  $\alpha$ -[[[2-(4-chlorophenyl)-1,4-dihydro-4-oxo-5-pyrimidinyl]amino]carbonyl]amino]-4-hydroxy-, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

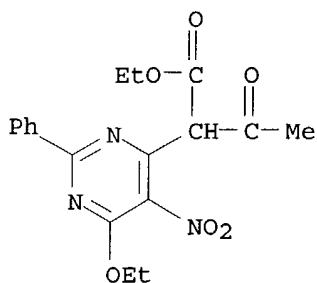


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L10 ANSWER 42 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1980:41984 CAPLUS  
DOCUMENT NUMBER: 92:41984  
TITLE: 2-Phenyl-4-hydroxy-6-methylpyrrolo[3,2-d]pyrimidine  
INVENTOR(S): Sokolova, V. N.; Novitskii, K. Yu.  
PATENT ASSIGNEE(S): Ordzhonikidze, S., All-Union Scientific-Research  
Chemical-Pharmaceutical Institute, USSR  
SOURCE: U.S.S.R. From: Otkrytiya, Izobret., Prom. Obraztsy,  
Tovarnye Znaki 1979, (37), 90.  
CODEN: URXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Russian  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

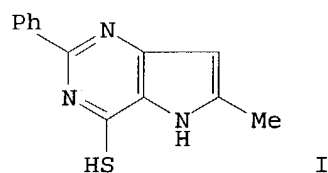
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
SU 690016	T	19791005	SU 1977-2521258	19770803
PRIORITY APPLN. INFO.:			SU 1977-2521258	19770803
AB Title compound was prepared by reacting 2-phenyl-4-ethoxy-5-nitro-6-[1-(ethoxycarbonyl)-2-oxopropyl]pyrimidine with Zn in HOAc at 60-90° followed by refluxing the resulting 2-phenyl-4-ethoxy-6-methyl-7-(ethoxycarbonyl)pyrrolo[3,2-d]pyrimidine with HCl.				
IT 72168-65-1				
RL: RCT (Reactant); RACT (Reactant or reagent) (reductive cyclization of)				
RN 72168-65-1 CAPLUS				
CN 4-Pyrimidineacetic acid, α-acetyl-6-ethoxy-5-nitro-2-phenyl-, ethyl ester (9CI) (CA INDEX NAME)				



L10 ANSWER 43 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1980:15521 CAPLUS  
DOCUMENT NUMBER: 92:15521  
TITLE: Study of pyrrolo[3,2-d]pyrimidine. III

09/ 811,359

AUTHOR(S): Sokolova, V. N.; Modnikova, G. A.; Novitskii, K. Yu.;  
Kravchenko, A. I.; Chernov, V. A.; Shcherbakova, L.  
I.; Pershin, G. N.  
CORPORATE SOURCE: Vses. Nauchno-Issled. Khim.-Farm. Inst., Moscow, USSR  
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1979), 13(9),  
17-22  
CODEN: KHFZAN; ISSN: 0023-1134  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
OTHER SOURCE(S): CASREACT 92:15521  
GI

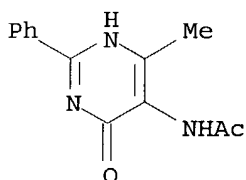


AB 2-Phenyl-4-mercapto-6-methylpyrrolo[3,2-d]pyrimidine (I) [72168-74-2] inhibited growth of *Lactobacillus casei* in vitro at 1-10 µg/mL and of *Mycobacterium tuberculosis* at 4 µg/mL. In expts. in vivo, I was active against sarcoma in mice and rats, but not against leukemia in mice. The other 6 4-alkylamino-2-phenyl-6-methylpyrrolo[3,2-d]pyrimidines and 11 4-alkyl(aralkyl)thio-2-phenyl-6-methylpyrrolo[3,2-d]pyrimidines prepared and tested showed no antibacterial activity, with the exception of 4-isobutylamino-2-phenyl-6-methylpyrrolo[3,2-d]pyrimidine [72168-70-8] which was weakly active.

IT **72168-63-9P**  
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
(preparation and cyclization of)

RN 72168-63-9 CAPLUS

CN Acetamide, N-(1,4-dihydro-6-methyl-4-oxo-2-phenyl-5-pyrimidinyl)- (9CI)  
(CA INDEX NAME)

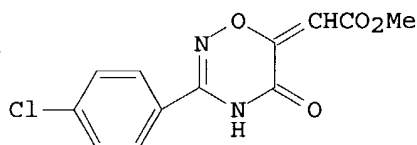


L10 ANSWER 44 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1979:420462 CAPLUS  
DOCUMENT NUMBER: 91:20462  
TITLE: Synthesis of 1,2,4-oxadiazines and their rearrangement to pyrimidines  
AUTHOR(S): Santilli, Arthur A.; Scotese, Anthony C.  
CORPORATE SOURCE: Res. Dev. Div., Wyeth Lab., Inc., Radnor, PA, 19087, USA  
SOURCE: Journal of Heterocyclic Chemistry (1979), 16(2), 213-16  
CODEN: JHTCAD; ISSN: 0022-152X  
DOCUMENT TYPE: Journal  
LANGUAGE: English

09/ 811,359

OTHER SOURCE(S) :  
GI

CASREACT 91:20462



I

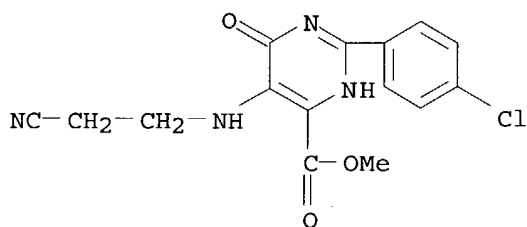
AB Several amide oximes underwent condensation reactions with MeO2CC.tplbond.CC(=O)OMe to give 1:1 adducts. Under basic conditions, these adducts underwent ring closure to give several Me [3-(substituted)-4,5-dihydro-5-oxo-6H-1,2,4-oxadiazin-6-ylidene]acetates, e.g. I. The reactions of these compds. with a variety of amines resulted in addition-rearrangement reactions with the formation of the corresponding Me 2-substituted-5-substituted amino-1,6-dihydro-6-oxo-4-pyrimidinecarboxylates.

IT 70274-26-9P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 70274-26-9 CAPLUS

CN 4-Pyrimidinecarboxylic acid, 2-(4-chlorophenyl)-5-[(2-cyanoethyl)amino]-1,6-dihydro-6-oxo-, methyl ester (9CI) (CA INDEX NAME)



L10 ANSWER 45 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1979:49472 CAPLUS

DOCUMENT NUMBER: 90:49472

TITLE: Relation between the chemical structure and stimulating activity of some nitro-, hydroxy-, and amino-substituted pyrimidines as illustrated by mono- and dicotyledonous plants

AUTHOR(S): Vladimirtsev, I. F.; Borisenko, V. P.; Boldyrev, I. V.; Nasyr, I. A.

CORPORATE SOURCE: Inst. Org. Khim., Kiev, USSR

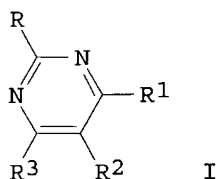
SOURCE: Fiziologicheskii Aktivnye Veshchestva (1978), 10, 45-7  
CODEN: FAVUAI; ISSN: 0533-1153

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI

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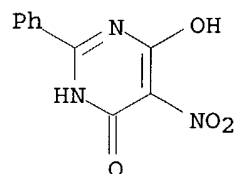
AB Of 17 title compds. I (R = H, Me, Ph, OH, or NH<sub>2</sub>; R1 = H, Cl, or OH; R2 = NH<sub>2</sub>, H, NO<sub>2</sub>, NHCOCO<sub>2</sub>Et, or NHAc; R3 = H, OH, or Me) 5-aminopyrimidine [591-55-9] and 4-methyl-6-hydroxypyrimidine [3524-87-6] most effectively stimulated the growth of lettuce and oats. Synthesis was given.

IT 68905-99-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and plant-growth stimulating activity of)

RN 68905-99-7 CAPLUS

CN 4(1H)-Pyrimidinone, 6-hydroxy-5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 46 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1979:7589 CAPLUS

DOCUMENT NUMBER: 90:7589

TITLE: Polycyclic compounds

INVENTOR(S): Dunkelmann, Guenter

PATENT ASSIGNEE(S): BASF A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 27 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

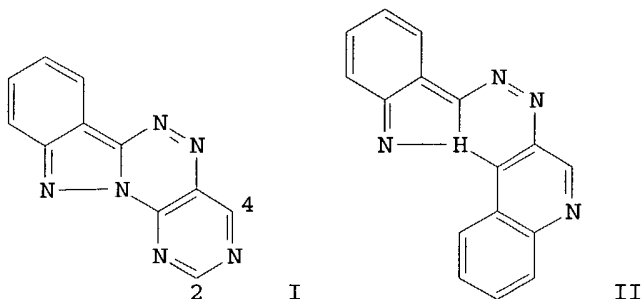
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2707710	A1	19780824	DE 1977-2707710	19770223
GB 1596690	A	19810826	GB 1978-7022	19780222
JP 54060328	A2	19790515	JP 1978-19179	19780223
PRIORITY APPLN. INFO.:			DE 1977-2707710	19770223

GI

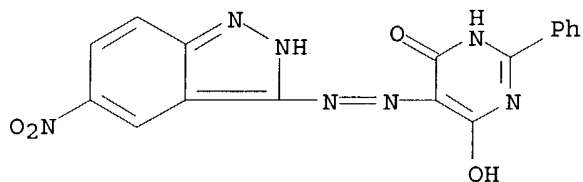


AB Polycyclic dyes containing substituted I and II nuclei were prepared and used to dye polyester fiber and PVC [9002-86-2] fast yellow shades. Thus, 3-aminoindazole → 2-phenyl-4,6-dihydroxypyrimidine [68386-19-6] was cyclized by heating in HOAc containing H<sub>2</sub>SO<sub>4</sub> to give I (2-Ph, 4-OH) [68386-18-5]. The other I and II were similarly prepared

IT 68386-06-1  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (cyclization of)

RN 68386-06-1 CAPLUS

CN 4(1H)-Pyrimidinone, 6-hydroxy-5-[(5-nitro-2H-indazol-3-yl)azo]-2-phenyl-  
 (9CI) (CA INDEX NAME)



L10 ANSWER 47 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1977:78554 CAPLUS

DOCUMENT NUMBER: 86:78554

TITLE: Hair dyeing agent

INVENTOR(S): Kubersky, Hans P.

PATENT ASSIGNEE(S): Henkel und Cie. G.m.b.H., Fed. Rep. Ger.

SOURCE: Ger. Offen., 13 pp.  
 CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

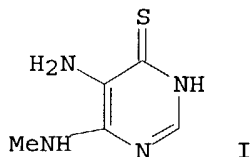
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2523045	A1	19761202	DE 1975-2523045	19750524
PRIORITY APPLN. INFO.:			DE 1975-2523045	19750524

GI

09/ 811,359



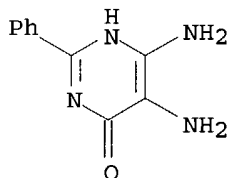
AB Diaminopyrimidine derivs. are developer components for oxidative dyeing of hair which provide a wide range of color nuances, are water soluble, are toxicol. and dermatol. innocuous, and have good fastness. For example, a dye cream was prepared containing (I) [61595-49-1] as developer and m-diaminoanisole as coupler. Gray hair treated with this cream developed an orange-brown color when oxidized with air and a brown color when oxidized with 1° H2O2.

IT 61595-45-7

RL: BIOL (Biological study)  
(as dye, for hair)

RN 61595-45-7 CAPLUS

CN 4(1H)-Pyrimidinone, 5,6-diamino-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 48 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1977:55486 CAPLUS

DOCUMENT NUMBER: 86:55486

TITLE: Azapurinones

INVENTOR(S): Broughton, Barbara J.; Large, Bryan J.; Marshall, Stuart Malcolm; Pain, David L.; Wooldridge, Kenneth R. H.

PATENT ASSIGNEE(S): May and Baker Ltd., UK

SOURCE: Ger. Offen., 34 pp. Addn. to Ger. Offen. 2,162,096.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

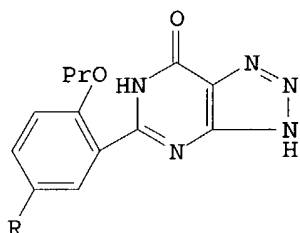
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2618694	A1	19761111	DE 1976-2618694	19760428
GB 1493685	A	19771130	GB 1975-17573	19750428
US 4039544	A	19770802	US 1976-680444	19760426
BE 841181	A4	19761027	BE 1976-166501	19760427
ZA 7602489	A	19770427	ZA 1976-2489	19760427
CA 1077933	A1	19800520	CA 1976-251095	19760427
NL 7604548	A	19761101	NL 1976-4548	19760428
PRIORITY APPLN. INFO.:			GB 1975-17573	19750428
			GB 1975-23785	19750602
			GB 1970-59552	19701215
			GB 1970-59556	19701215
			GB 1971-49756	19711026

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GB 1971-53457	19711117
US 1971-207986	19711214
US 1973-364425	19730529

GI



I

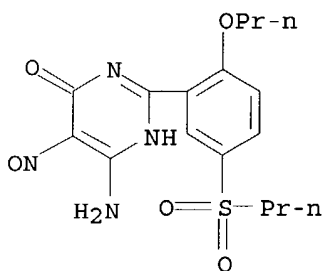
AB 3,6-Dihydro-7H-v-triazolo[4,5-d]pyrimidin-7-ones (I; R = MeO<sub>2</sub>C, EtO<sub>2</sub>C, BuO<sub>2</sub>C, BuS, BuSO, MeSO<sub>2</sub>, PrSO<sub>2</sub>, Me<sub>2</sub>CHSO<sub>2</sub>, BuSO<sub>2</sub>, Me<sub>2</sub>CHCH<sub>2</sub>SO<sub>2</sub>), useful in treatment of bronchial asthma (no data), are prepared by reaction of 5,6-diamino-2-phenyl-4(3H)-pyrimidinones with HNO<sub>2</sub>. The diaminopyrimidinones are obtained from 5-nitroso-6-aminopyrimidinones which are prepared from the 2-propoxybenzamides via the benzamidines. Thus, reaction of 15 % 5,6-diamino-2-[2-propoxy-5-(propylsulfonyl)phenyl]-4(3H)-pyrimidinone with NaNO<sub>2</sub> in aqueous HCl at 0°, followed by stirring 2 hr at 0° and 18 hr at room temperature, gives 12 g I (R = PrSO<sub>2</sub>).

IT 61627-25-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, and diaminopyrimidinone from)

RN 61627-25-6 CAPLUS

CN 4(1H)-Pyrimidinone, 6-amino-5-nitroso-2-[2-propoxy-5-(propylsulfonyl)phenyl]- (9CI) (CA INDEX NAME)



L10 ANSWER 49 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1977:5410 CAPLUS

DOCUMENT NUMBER: 86:5410

TITLE: A new, general synthesis of purines

AUTHOR(S): Yoneda, Fumio; Nagamatsu, Tomohisa

CORPORATE SOURCE: Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, Japan

SOURCE: Journal of the Chemical Society, Perkin Transactions  
1: Organic and Bio-Organic Chemistry (1972-1999)  
(1976), (14), 1547-50

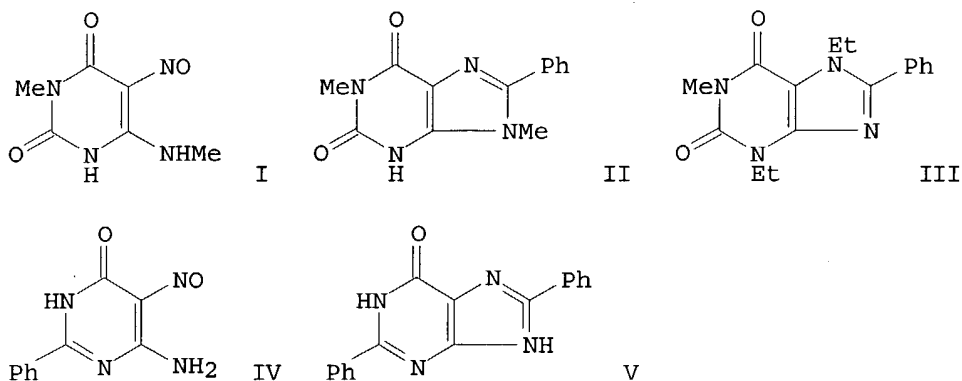
CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 86:5410

GI



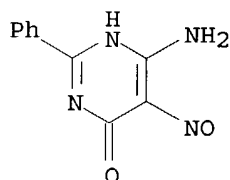
AB 6-Amino-5-nitrosouracil derivs. underwent cyclocondensation reactions with  $\text{RCH:NNMe}_2$ , prepared in situ by reaction of  $\text{RCHO}$  with  $\text{NH}_2\text{NMe}_2$ , to give the corresponding xanthine derivs. Thus, the uracil I with  $\text{PhCH:NNMe}_2$  in DMF gave 71% II. Alkylation of 9-substituted 1-methylxanthines with excess alkyl halide in DMF in the presence of  $\text{K}_2\text{CO}_3$  gave the corresponding 3,7-dialkyl-1-methylxanthine, with elimination of the 9-substituent. Thus, II with EtI and  $\text{K}_2\text{CO}_3$  in DMF gave 68% III. Similar treatment of 6-amino-4-hydroxy-5-nitroso-2-phenylpyrimidines with  $\text{RCH:NNMe}_2$  gave the corresponding purines. Thus, the pyrimidine IV with  $\text{PhCH:NNMe}_2$  in DMF gave 49% purine V.

IT 5466-66-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclocondensation reaction with benzaldehyde dimethylhydrazone)

RN 5466-66-0 CAPLUS

CN 4(1H)-Pyrimidinone, 6-amino-5-nitroso-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 50 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1975:572422 CAPLUS

DOCUMENT NUMBER: 83:172422

TITLE: Antiallergic activity of 2-phenyl-8-azapurin-6-ones

AUTHOR(S): Broughton, B. J.; Chaplen, P.; Knowles, P.; Lunt, E.;  
Marshall, S. M.; Pain, D. L.; Wooldridge, K. R. H.

CORPORATE SOURCE: Res. Lab., May and Baker Ltd., Dagenham/Essex, UK

SOURCE: Journal of Medicinal Chemistry (1975), 18(11), 1117-22  
CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 83:172422

GI For diagram(s), see printed CA Issue.

AB The cycloaddn. reaction of benzamidines with Et cyanonitrosoacetate [5457-25-0] gave aminophenylnitrosopyrimidinones which underwent reduction, nitrosation, and cyclization to give 44 title azapurinones. The azapurinones had varying antiallergic activity in the rat passive cutaneous anaphylactic reaction with 2-(o-propoxyphenyl)-8-azapurin-6-one (I) [37762-06-4] being 40 times more potent than disodium cromoglycate



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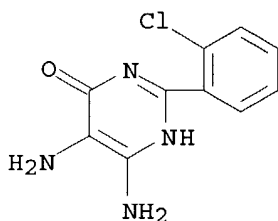
[15826-37-6]. Structure activity relations were discussed.

IT 57075-30-6P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation and cycloaddn. with sodium nitrate)

RN 57075-30-6 CAPLUS

CN 4(1H)-Pyrimidinone, 5,6-diamino-2-(2-chlorophenyl)- (9CI) (CA INDEX NAME)



L10 ANSWER 51 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1974:505449 CAPLUS

DOCUMENT NUMBER: 81:105449

TITLE: Novel synthetic route to heterocycles via  
intramolecular cycloaddition of azalogs of hexatriene.  
New syntheses of purines and pyrazolo[3,4-  
d]pyrimidines

AUTHOR(S): Yoneda, Fumio; Higuchi, Masatsugu; Nagamatsu, Tomohisa  
CORPORATE SOURCE: Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, Japan  
SOURCE: Journal of the American Chemical Society (1974),  
96(17), 5607-8

CODEN: JACSAT; ISSN: 0002-7863

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

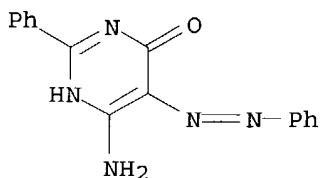
AB The thermolysis of 5-(arylo)-1,3-dimethyl-6-  
[[dimethylamino)methylene]amino]-uracils gave 8-  
(dimethylamino)theophylline and 5-aryl-1,3-dimethyl-7-(dimethylamino)-  
5,6(or 5,8)-dihydro-6-azaluminazines. The reaction of 6-amino-1,3-dimethyl-  
5-(phenylazo)uracil with aromatic aldehydes gave the corresponding  
8-aryltheophyllines and 5-aryl-1,3-dimethyl-7-phenyl-5,6(or  
5,8)-dihydro-6-azaluminazines. This purine synthesis is applicable to other  
6-amino-5-(phenylazo)pyrimidines such as 6-amino-1-methyl-5-  
(phenylazo)uracil and 6-amino-4-hydroxy-2-phenyl-5-(phenylazo)pyrimidine  
to give the resp. purine derivs. Heating 6-(benzylidene-hydrazino)uracil  
derivs. with aromatic aldehydes in DMF gave the corresponding  
3-aryl-2-benzylpyrazolo[3,4-d] pyrimidine-4,6(5H,-7H)-diones I in  
excellent yields.

IT 54014-72-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
(condensation with aromatic aldehydes)

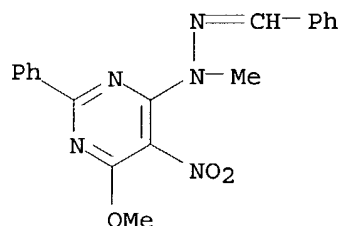
RN 54014-72-1 CAPLUS

CN 4(1H)-Pyrimidinone, 6-amino-2-phenyl-5-(phenylazo)- (9CI) (CA INDEX NAME)

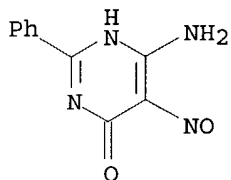


09/ 811,359

L10 ANSWER 52 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1974:477865 CAPLUS  
DOCUMENT NUMBER: 81:77865  
TITLE: Photochemical synthesis of condensed triazole N-oxide  
AUTHOR(S): Maki, Yoshifumi; Suzuki, Mikio; Izuta, Keiji; Iwai, Shunji  
CORPORATE SOURCE: Gifu Coll. Pharm., Gifu, Japan  
SOURCE: Chemical & Pharmaceutical Bulletin (1974), 22(6), 1269-74  
CODEN: CPBTAL; ISSN: 0009-2363  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI For diagram(s), see printed CA Issue.  
AB Photolysis of the uracil I (R = H) in C<sub>6</sub>H<sub>6</sub> gave the pyrazolopyrimidine II and the triazolopyrimidine oxide III. Photolysis of I (R = Me) in MeCN at 338 mμ gave III exclusively.  
IT 53246-62-1  
RL: RCT (Reactant); RACT (Reactant or reagent) (photolysis of)  
RN 53246-62-1 CAPLUS  
CN Benzaldehyde, (6-methoxy-5-nitro-2-phenyl-4-pyrimidinyl)methylhydrazone (9CI) (CA INDEX NAME)



L10 ANSWER 53 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1973:466312 CAPLUS  
DOCUMENT NUMBER: 79:66312  
TITLE: New synthesis of substituted 8-aminopurine derivatives  
AUTHOR(S): Yoneda, Fumio; Higuchi, Masatsugu; Matsumura, Takafumi; Senga, Keitaro  
CORPORATE SOURCE: Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, Japan  
SOURCE: Bulletin of the Chemical Society of Japan (1973), 46(6), 1836-9  
CODEN: BCSJA8; ISSN: 0009-2673  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
GI For diagram(s), see printed CA Issue.  
AB The treatment of 6-amino-5-nitrosopyrimidinediones with Vilsmeier-type reagents (substituted formamides and phosphorus oxychloride) afforded substituted 8-aminopurines (I, R = NMe<sub>2</sub>, NEt<sub>2</sub>, NHMe, NMePh). However, the treatment of 6-amino-4-hydroxy-2-methyl-5-nitrosopyrimidine with the same reagents gave 2-(chloromethyl)-8-(dimethylamino)-6-hydroxypurine.  
IT 5466-66-0  
RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with formamides)  
RN 5466-66-0 CAPLUS  
CN 4(1H)-Pyrimidinone, 6-amino-5-nitroso-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 54 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1972:539952 CAPLUS

DOCUMENT NUMBER: 77:139952

TITLE: Formation of new mesoionic pyrimidines

AUTHOR(S): Maki, Y.; Sako, M.; Suzuki, M.

CORPORATE SOURCE: Gifu Coll. Pharm., Gifu, Japan

SOURCE: Journal of the Chemical Society, Chemical Communications (1972), (17), 999-1000  
CODEN: JCCCAT; ISSN: 0022-4936

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

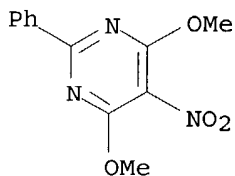
AB Pyrolysis of 4,6-dimethoxy-5-nitropyrimidine (I) at 200° for 15 min gave 70% anhydro-4-hydroxy-1,3-dimethyl-5-nitro-6-oxopyrimidinium (II) hydrochloride and 1-methyl-4-methoxy-5-nitro-6(1H)-pyrimidinone which at 200° gave II. Similarly the 2-phenyl derivative of I gave the corresponding pyrimidinium (III) hydrochloride (80%) and pyrimidinone which at 200° gave III. II or III with boiling aqueous KOH gave MeHNCO<sup>+</sup>(NO<sub>2</sub>):C(OH)NHMe quant. Pyrolysis of 4,6-dimethoxy-2-phenylpyrimidine caused O → N alkyl migration to give the corresponding N-alkyl derivs.

IT 29939-35-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
(pyrolysis of)

RN 29939-35-3 CAPLUS

CN Pyrimidine, 4,6-dimethoxy-5-nitro-2-phenyl- (8CI, 9CI) (CA INDEX NAME)



L10 ANSWER 55 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1972:501508 CAPLUS

DOCUMENT NUMBER: 77:101508

TITLE: Structure of aroyl isocyanide trimers

AUTHOR(S): Douchis, Harry

CORPORATE SOURCE: Chem. Res. Dev. Cent., FMC Corp., Princeton, NJ, USA

SOURCE: Journal of Organic Chemistry (1972), 37(16), 2583-7  
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The structure of the trimer of benzoyl isocyanide, prepared by the action of AgCN on BzBr, is 7-benzoylimino-2,5-diphenyloxazolo[5,4-d]pyrimidin-7-one. The scope and limitation of the trimerization reaction is discussed.

IT 34906-02-0P

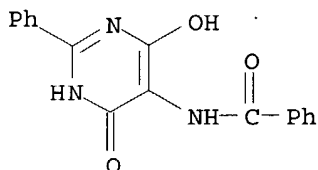
RL: SPN (Synthetic preparation); PREP (Preparation)

09/ 811,359

(preparation of)

RN 34906-02-0 CAPLUS

CN Benzamide, N-(1,4-dihydro-6-hydroxy-4-oxo-2-phenyl-5-pyrimidinyl)- (9CI)  
(CA INDEX NAME)



L10 ANSWER 56 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1972:488766 CAPLUS

DOCUMENT NUMBER: 77:88766

TITLE: Syntheses of some androstano[2,3-g]pteridines

AUTHOR(S): Yoneda, Fumio; Fukazawa, Shinobu; Nishigaki, Sadao

CORPORATE SOURCE: Fac. Pharm. Sci., Kumamoto Univ., Kumamoto, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1972), 20(7),  
1428-31

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

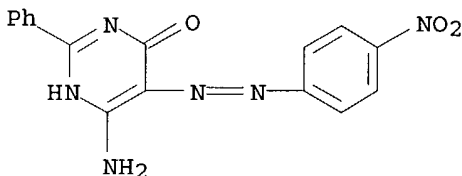
AB Morpholino and pyrrolidino derivs. of 17 $\beta$ -hydroxy-5 $\alpha$ -androstano-3-one reacted with 6-amino-5-nitrosopyrimidines or 6-amino-5-phenylazo-pyrimidines to give the corresponding androstano [2,3-g] pteridines. These steroidal pteridines were also prepared by the Isay pteridine synthesis from 17 $\beta$ -hydroxy-5 $\alpha$ -androstane-2,3-dione and the corresponding 5,6-diaminopyrimidines.

IT 38522-17-7P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 38522-17-7 CAPLUS

CN 4(1H)-Pyrimidinone, 6-amino-5-[(4-nitrophenyl)azo]-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 57 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1972:46170 CAPLUS

DOCUMENT NUMBER: 76:46170

TITLE: Pteridines. XXVI. Preparation and properties of some 3,4- and 5,6-dihydropteridines

AUTHOR(S): Taylor, Edward C.; Thompson, Malcolm J.; Perlman, Katherine; Mengel, Rudolf; Pfleiderer, Wolfgang

CORPORATE SOURCE: Dep. Chem., Princeton Univ., Princeton, NJ, USA

SOURCE: Journal of Organic Chemistry (1971), 36(26), 4012-25

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Treatment of 8-alkyl-7(8H)-pteridinone-6-carboxylic acid derivs.

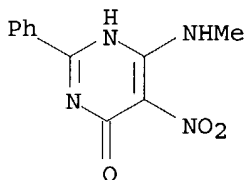
(substituted at position 4 with H or Me) with NaBH<sub>4</sub> gives bright yellow dihydro compds. which are 10,000 times weaker acids, and exhibit uv absorption maxima some 50-60 nm higher, than the starting pteridinones. The influence of 2 and 4-substituents on this reduction was carefully examined, and evaluation of both spectroscopic (uv, ir, and NMR) and chemical data has shown that these reduction products are 3,4-dihydro derivs., and not 4,8- (or 5,8-) dihydro derivs. as previously suggested. By contrast, catalytic reduction of the same series of 8-alkyl-7(8H)-pteridinone-6-carboxylic acids and esters gave 5,6-dihydro compds. with different chemical and phys. properties. 3,4-Dihydro compds. rearrange quant. and irreversibly to the 5,6-dihydro isomers in F<sub>3</sub>CCO<sub>2</sub>H.

IT 31937-03-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 31937-03-8 CAPLUS

CN 4(1H)-Pyrimidinone, 6-(methylamino)-5-nitro-2-phenyl- (9CI) (CA INDEX  
NAME)



L10 ANSWER 58 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1971:510265 CAPLUS

DOCUMENT NUMBER: 75:110265

TITLE: Reaction of 4,6-dimethoxy-5-nitropyrimidine with  
methylhydrazine. Formation of 4-hydrazine-6-  
hydroxypyrimidine

AUTHOR(S): Christensen, Bert E.; Stahl, Quade; Lehmkuhl, Frank

CORPORATE SOURCE: Dep. Chem., Oregon State Univ., Corvallis, OR, USA

SOURCE: Journal of Organic Chemistry (1971), 36(17), 2462-6  
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 75:110265

AB Reaction of 4,6-dimethoxy-5-nitropyrimidine (I) with MeNHNH<sub>2</sub> in refluxing pyridine or BuOH involves methylation of the solvent by I and the nucleophilic substitution and demethylation of the methylhydrazino substituent in the 5 position to yield 4-hydrazino-6-hydroxypyrimidine. The first step in this sequence of reactions involves the methylation of the solvent, followed by nucleophilic substitution of methylhydrazine in the 4 position, migration of its Me substituent to form C to O bond with the adjacent nitro substituent, and eventual elimination of Me nitrite from the 5 position as one of the reaction products. 4,6-Dimethoxy-5-nitropyrimidine reacts with pyridine (in the absence of MeNHNH<sub>2</sub>) to yield an insol. methylpyridium salt which is not a precursor of 4-hydrazino-6-hydroxypyrimidine. The mother liquor from this reaction on acid hydrolysis yields 4-hydroxy-6-methoxy-5-nitropyrimidine and reacts with MeNHNH<sub>2</sub> to yield 4-hydroxy-6-hydrazinopyrimidine. Both 4-chloro-6-hydroxy-5-nitropyrimidine and 4,6-dichloro-5-nitropyrimidine react with MeNHNH<sub>2</sub> in alc. to yield the corresponding methylhydrazino derivs.

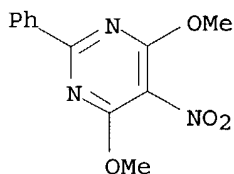
IT 29939-35-3P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 29939-35-3 CAPLUS

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CN Pyrimidine, 4,6-dimethoxy-5-nitro-2-phenyl- (8CI, 9CI) (CA INDEX NAME)



L10 ANSWER 59 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1971:112015 CAPLUS

DOCUMENT NUMBER: 74:112015

TITLE: New synthesis of alloxazines

AUTHOR(S): Yoneda, Fumio; Ichiba, Misuzu; Ogiwara, Kazuko; Nishigaki, Sadao

CORPORATE SOURCE: Sch. Med., Keio Univ., Tokyo, Japan

SOURCE: Journal of the Chemical Society [Section] D: Chemical Communications (1971), (1), 23  
CODEN: CCJDAO; ISSN: 0577-6171

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

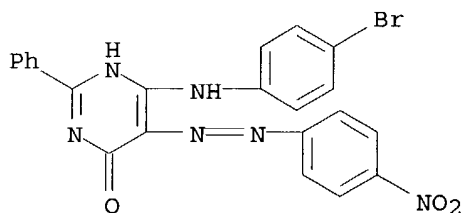
AB 2-Phenyl-2-deoxyalloxazine (I, R = H) and its 7-chloro (I, R = Cl) and 7-bromo derivative (I, R = Br) were prepared by cyclization of II (R = H, Cl, Br) with 10% H<sub>2</sub>SO<sub>4</sub> in HOAc. Using 20% H<sub>2</sub>SO<sub>4</sub>, HOAc alone, or F<sub>3</sub>CCO<sub>2</sub>H alone did not lead to cyclization. 5-Chlorophenylazo- and 5-phenylazo-6-anilino-4-hydroxy-2-phenylpyrimidine could not be cyclized by this method. II were prepared by treating 6-amino-2-phenyl-4-hydroxypyrimidine with p-RC<sub>6</sub>H<sub>4</sub>NH<sub>2</sub> and then coupling with p-nitrobenzenediazonium chloride.

IT 31595-55-8P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 31595-55-8 CAPLUS

CN 4(3H)-Pyrimidinone, 6-(p-bromoanilino)-5-[(p-nitrophenyl)azo]-2-phenyl- (8CI) (CA INDEX NAME)



L10 ANSWER 60 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1971:111997 CAPLUS

DOCUMENT NUMBER: 74:111997

TITLE: Oxidation of 5-nitrosopyrimidines by nitrous acid. A synthesis of 5-nitropyrimidines

AUTHOR(S): Nishigaki, Sadao; Ogiwara, Kazuko; Yoneda, Fumio

CORPORATE SOURCE: Sch. Med., Keio Univ., Tokyo, Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1971), 19(2), 418-19

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal

LANGUAGE: English

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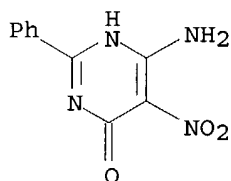
AB Some 2,4,6-trisubstituted pyrimidines gave with NaNO<sub>2</sub> in H<sub>2</sub>SO<sub>4</sub> the corresponding 5-nitropyrimidines, by way of nitrosation. Thus, 2-phenyl-4-hydroxy-6-morpholinopyrimidine gave 2-phenyl-4-hydroxy-5-nitro-6-morpholinopyrimidine.

IT 23120-15-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 23120-15-2 CAPLUS

CN 4-Pyrimidinol, 6-amino-5-nitro-2-phenyl- (8CI) (CA INDEX NAME)



L10 ANSWER 61 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1969:449899 CAPLUS

DOCUMENT NUMBER: 71:49899

TITLE: Heterocyclic studies. VIII. 2-Phenylpteridine and some related compounds

AUTHOR(S): Clark, Jim; Murdoch, P. N. T.; Roberts, D. L.

CORPORATE SOURCE: Univ. Salford, Salford, UK

SOURCE: Journal of the Chemical Society [Section] C: Organic (1969), (10), 1408-12

CODEN: JSOAX; ISSN: 0022-4952

DOCUMENT TYPE: Journal

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

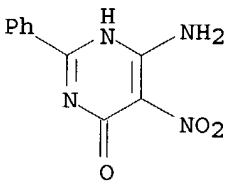
AB Syntheses of 2-phenylpteridine (I) and its 4- and 7-monomethyl, 4,7- and 6,7-dimethyl, and 4,6,7-trimethyl derivs. are described. Oxidation of 2-phenyl-, 7-methyl-2-phenyl-, and 6,7-dimethyl-2-phenylpteridines with H<sub>2</sub>O<sub>2</sub> in acetic acid gave the corresponding 4-hydroxy derivs. Further oxidation of 4-hydroxy-2-phenylpteridine gave 4,6,7-trihydroxy-2-phenylpteridine. In acid solution, 2-phenylpteridine gave a mixture of 3,4-monohydrated and 5,6,7,8-dihydrated cations which rapidly changed to a solution almost free of the monohydrate. 4-Methyl- and 4,7-dimethyl-2-phenylpteridines also gave essentially all 5,6,7,8-dihydrated cations but mainly 3,4-hydrated species were present in the equilibrium mixts. of cations formed from 7-methyl- and 6,7-dimethyl-2-phenylpteridine. <sup>1</sup>H N.M.R. and uv spectra and pK<sub>a</sub> values are recorded.

IT 23120-15-2P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

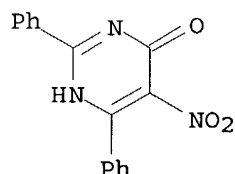
RN 23120-15-2 CAPLUS

CN 4-Pyrimidinol, 6-amino-5-nitro-2-phenyl- (8CI) (CA INDEX NAME)



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L10 ANSWER 62 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1969:11661 CAPLUS  
DOCUMENT NUMBER: 70:11661  
TITLE: Syntheses of 4,5-disubstituted 2,6-diarylpyrimidines  
AUTHOR(S): Weidinger, Hans; Sturm, Hans Juergen  
CORPORATE SOURCE: Farbenforschungslab., Bad. Anilin- und Soda-Fabrik  
A.-G., Ludwigshafen/Rhein, Fed. Rep. Ger.  
SOURCE: Justus Liebig's Annalen der Chemie (1968), 716, 143-6  
CODEN: JLACBF; ISSN: 0075-4617  
DOCUMENT TYPE: Journal  
LANGUAGE: German  
OTHER SOURCE(S): CASREACT 70:11661  
AB RCN reacted with SO3 to give 4,6-bis(R-substituted)-1,2,3,5-oxathiadiazine  
2,2-dioxides (I), which lose SO2 and add 2C fragments to give  
2,6-bis(R-substituted)-4-(R1-substituted)-5-(R2-substituted)-pyrimidines  
(II). Reaction of I with AcCH2CO2Et gave II (R = Ph, R1 = OH, R2 =  
CO2Et); treatment of I with CH2(CN)CO2Et gave II (R = Ph, R1 = OH, R2 =  
CN); CH2(CN)2 and I gave II (R = Ph or p-MeC6H4, R1 = NH2, R2 = CN), while  
1-morpholinocyclohexene led to 2,4-diphenyl-5,6,7,8-tetrahydro-  
quinazoline.  
IT 20954-88-5P  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
RN 20954-88-5 CAPLUS  
CN 4-Pyrimidinol, 5-nitro-2,6-diphenyl- (8CI) (CA INDEX NAME)



L10 ANSWER 63 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1968:49645 CAPLUS  
DOCUMENT NUMBER: 68:49645  
TITLE: 4-Amino-5-arylazopyrimidine derivatives  
INVENTOR(S): Fujimoto, Yasuo; Teranishi, Masayuki  
PATENT ASSIGNEE(S): Kyowa Fermentation Industry Co., Ltd.  
SOURCE: Jpn. Tokkyo Koho, 4 pp.  
CODEN: JAXXAD  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 42008388	B4	19670411	JP	19631228

AB A mixture of 4.35 g. Et 2-phenylazocynoacetate, 80 ml. EtOH, 0.42 g. Na, and 1.55 g. thiourea is refluxed 2 hrs., cooled, and neutralized with AcOH and the product recrystd. (EtOH-pyridine) to give 3.5 g. 2-mercapto-4-amino-5-phenylazo-6-pyrimidinol. Similarly prepared are 4-amino-2,6-dihydroxy-5-(p-hydroxyphenylazo)pyrimidine, 2,4-diamino-5-(p-methylphenylazo)-6-hydroxypyrimidine, 4-amino-5-(m-nitrophenylazo)-6-hydroxy-2-methylpyrimidine, 4-amino-6-hydroxy-5-phenylazo-2-(methylthio)pyrimidine, 4-amino-5-phenylazo-6-hydroxypyridine, 4-amino-6-hydroxy-2-phenyl-5-(p-methoxyphenylazo)pyridine, 4-amino-2-(p-chlorophenyl)-6-hydroxy-5-(m-carboxyphenylazo)pyrimidine, 4-amino-6-hydroxy-5-(p-



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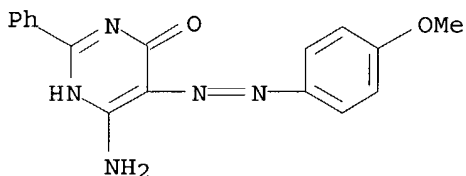
sulfophenylazo)-2-(methylthio)pyrimidine, 4-amino-2-ethoxy-6-hydroxy-5-(o-chlorophenylazo)pyrimidine, 4-amino-6-hydroxy-2-pyridyl- 5 - (m - methylphenylazo) - 1 - methylpyrimidine, and 4-amino-6-hydroxy-5-(p-nitrophenylazo)-2-benzylpyrimidine. The products are intermediates for the manufacture of condiments and pharmaceuticals.

IT 17041-99-5P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 17041-99-5 CAPLUS

CN 4-Pyrimidinol, 6-amino-5-[(p-methoxyphenyl)azo]-2-phenyl- (8CI) (CA INDEX NAME)



L10 ANSWER 64 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1965:9095 CAPLUS

DOCUMENT NUMBER: 62:9095

ORIGINAL REFERENCE NO.: 62:1651d-e

TITLE: Syntheses of 4-hydroxy-5-nitropyrimidines

AUTHOR(S): Simchen, G.

CORPORATE SOURCE: Tech. Hochschule, Stuttgart, Germany

SOURCE: Angew. Chem. (1964), 76(20), 860

DOCUMENT TYPE: Journal

LANGUAGE: German

OTHER SOURCE(S): CASREACT 62:9095

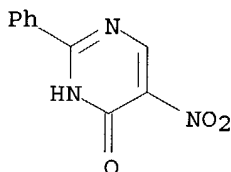
GI For diagram(s), see printed CA Issue.

AB Condensation of MeNO<sub>2</sub> with HC(OEt)<sub>2</sub>-NMe<sub>2</sub> (I) 5 hrs. at 60° afforded Me<sub>2</sub>NCH:CHNO<sub>2</sub>, which added to PhCONCO over 12 hrs. at 20° to give Me<sub>2</sub>NCH:C(NO<sub>2</sub>)-CONHCOPh, which in turn reacted with NH<sub>2</sub> in HCONMe<sub>2</sub> 1 hr. at 0° and subsequently 3 hrs. at 140° to give 4-hydroxy-5-nitro-2-phenylpyrimidine (II), m. 278°, in 42% yield calculated on MeNO<sub>2</sub>. Similarly, condensation of H<sub>2</sub>NCH:C(NO<sub>2</sub>)CONH<sub>2</sub> with I at 50° in EtOH gave 4-hydroxy-5-nitropyrimidine, m. 192°, in 20% yield.

IT 3749-46-0, 4-Pyrimidinol, 5-nitro-2-phenyl-  
(preparation of)

RN 3749-46-0 CAPLUS

CN 4(1H)-Pyrimidinone, 5-nitro-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 65 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1964:45728 CAPLUS

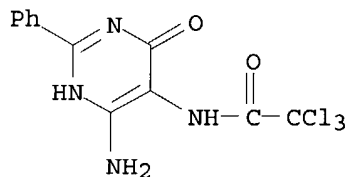
DOCUMENT NUMBER: 60:45728

ORIGINAL REFERENCE NO.: 60:8031c-e

TITLE: Formation of 6-hydroxypteridines by condensation of

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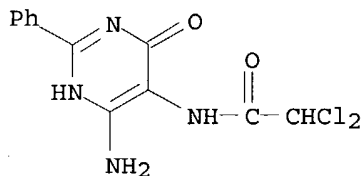
AUTHOR(S): 4,5-diaminopyrimidines with chloral  
Bergmann, F.; Tamari, M.; Ungar-Waron, Hanna  
CORPORATE SOURCE: Hebrew Univ., Jerusalem  
SOURCE: Journal of the Chemical Society, Abstracts (1964),  
(Feb.), 565-72  
CODEN: JCSAAZ; ISSN: 0590-9791  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
GI For diagram(s), see printed CA Issue.  
AB Chloral hydrate reacts with 4,5-diaminopyrimidines, bearing O at position  
6, to yield 6-hydroxypteridines (I). The ready elimination of all 3 Cl  
atoms in this condensation contrasts sharply with the resistance of the  
corresponding 5-di- and 5-trichloroacetamido derivs. to cyclization. It  
is assumed that the aldehyde group of chloral condenses first with the  
5-amino group, the latter then inducing formation of an aziridine ring.  
This ring opens with simultaneous chloride shift, to produce the  
chloroimido structure, N: CClCHClOH, in which the hemiacetal group readily  
condenses with the 4-amino group of the pyrimidine.  
IT 91492-97-6, 4-Pyrimidinol, 6-amino-2-phenyl-5-(2,2,2-  
trichloroacetamido)-  
(preparation of)  
RN 91492-97-6 CAPLUS  
CN 4-Pyrimidinol, 6-amino-2-phenyl-5-(2,2,2-trichloroacetamido)- (7CI) (CA  
INDEX NAME)



L10 ANSWER 66 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1964:45727 CAPLUS  
DOCUMENT NUMBER: 60:45727  
ORIGINAL REFERENCE NO.: 60:8031b-c  
TITLE: Reactions of nucleic acids and their components. III.  
Interaction of adenine and uracil with formaldehyde  
AUTHOR(S): Lewin, S.  
CORPORATE SOURCE: South-West Essex Tech. Coll., London  
SOURCE: Journal of the Chemical Society, Abstracts (1964),  
(Feb.), 792-809  
CODEN: JCSAAZ; ISSN: 0590-9791  
DOCUMENT TYPE: Journal  
LANGUAGE: Unavailable  
AB cf. CA 57, 2222f. The interactions of HCHO with adenine (I) and uracil  
(II) have been examined by using the pH-variation method and  
spectrophotometry in the temperature range 20-40°. The results with I  
are interpretable in terms of a major interaction of the unionized N-10  
amino group and a minor interaction with the corresponding cation, each  
with one mol. of HCHO. Evidence for reaction of HCHO with the N-9-H group  
of purines has been obtained spectrophotometrically. The acid imino group  
of II also reacts with 1 mol. of HCHO. The reactions of the neutral mols.  
are exothermic. New structural configurations, involving H-bonded  
hydrations of the nitrogenous groups of I and II are advocated.  
IT 91962-07-1, 4-Pyrimidinol, 6-amino-5-(2,2-dichloroacetamido)-2-  
phenyl-  
(preparation of)  
RN 91962-07-1 CAPLUS

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CN 4-Pyrimidinol, 6-amino-5-(2,2-dichloroacetamido)-2-phenyl- (7CI) (CA INDEX NAME)



L10 ANSWER 67 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1963:428556 CAPLUS

DOCUMENT NUMBER: 59:28556

ORIGINAL REFERENCE NO.: 59:5168e-g

TITLE: 2-Phenylpurines, their chemical and enzymological reactivity

AUTHOR(S): Bergmann, F.; Kalmus, A.; Ungar-Waron, H.; Kwietny-Govrin, H.

CORPORATE SOURCE: Hebrew Univ.-Hadassah Med. School, Jerusalem  
SOURCE: Journal of the Chemical Society, Abstracts (1963) 3729-35

CODEN: JCSAAZ; ISSN: 0590-9791

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

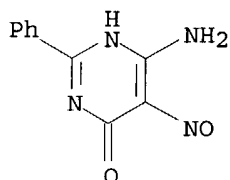
GI For diagram(s), see printed CA Issue.

AB 2-Phenylpurines (I) are accessible from 4,5-diamino-2-phenylpyrimidine and its 6-hydroxy and 6-mercapto derivs. Thiation of 2-phenylhypoxanthine proceeds as smoothly as that of hypoxanthine itself. 6,8-Dihydroxy-2-phenylpurine is thiated exclusively at position 6, in contrast to the corresponding 2-methyl derivative. Xanthine oxidase is unable to attack position 6 in 2-phenylpurine or its 8-hydroxy derivative, but does so without difficulty in the corresponding 2-methylpurines. 2-Phenylhypoxanthine is oxidized by the enzyme about 50 times faster than the 2-methyl derivative.

IT 5466-66-0, 4-Pyrimidinol, 6-amino-5-nitroso-2-phenyl- (preparation of)

RN 5466-66-0 CAPLUS

CN 4(1H)-Pyrimidinone, 6-amino-5-nitroso-2-phenyl- (9CI) (CA INDEX NAME)



L10 ANSWER 68 OF 68 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1953:72848 CAPLUS

DOCUMENT NUMBER: 47:72848

ORIGINAL REFERENCE NO.: 47:12395i,12396a-i

TITLE: Investigations of pterins. I. 2-Furyl-4-hydroxypterins

AUTHOR(S): Andrisano, Renato; Maioli, Lillia

CORPORATE SOURCE: Univ. Catania, Italy

SOURCE: Gazzetta Chimica Italiana (1953), 83, 264-8

CODEN: GCITA9; ISSN: 0016-5603

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

GI For diagram(s), see printed CA Issue.

AB In connection with expts. on the pharmacological activity of furyl derivs. (cf. Boll. sci. faculty chim. ind. Bologna 8, 321(1950); C.A. 45, 3851e), some derivs. of the type  $N:CAR.N:CH.C:C.N:CX.CX':N$  (I) (where X and X' may be H, OH, Me, Ph,  $MeC_6H_4$ , furyl, or methylfuryl) were prepared in order to establish the influence of the furyl group compared to that of the Ph group. To prepare the pterins, the reaction of Isay [Ber. 39, 250(1906)] was utilized; i.e., the 2-aryl-6-hydroxy-4,5-diaminopyrimidines were condensed with the o-dicarbonyl derivs., with 50-60% yields:

$$N:CAR.N:C(OH).C(NH_2):CNH_2 \text{ (II)} + (COX)_2 \rightarrow$$

$$N:CAR.N:C(OH).C:C.N:CX.CX':N \text{ (III)}.$$

The reactions were carried out in water, dilute AcOH, or concentrated AcOH, by refluxing 0.1 mole II and 0.11 mole diketone for 1-2 hrs. The II compds. were prepared in 3 steps [cf. Boll. accad. gioenia [4] 2, II(1952)]: (1) condensation of  $ArC(:NH)NH_2$  compds. with  $NCCH_2CO_2Et$  (IV) to  $N:CAR.N:C(OH).CH:CNH_2$  (V) compds. according to the procedure of Maggiolo, et al. (C.A. 46, 2551a); (2) coupling of V with  $PhN_2Cl$  (VI) to form  $N:CAR.N:C(OH).C(N:NPh):CNH_2$  (VII) compds., and (3) reduction of VII by the method of Benson, et al. (C.A. 44, 10717i) to II. I compds. are soluble in aqueous alkalis and insol. in inorg. acids. They can be well purified by AcOH. NaOMe (0.4 mole in 100 cc. MeOH), 0.1 mole  $NCCH_2CO_2Et$ , and 0.1 mole 2-furylamidine in MeOH, refluxed 2 hrs., distilled in vacuo, the residue taken up in a min. of water, acidified with AcOH, and the precipitate purified by water, yield approx. 58% of 2-furyl-4-amino-6-hydroxypyrimidine (VIII), m.  $290^\circ$ . VI (0.1 mole), added to 0.1 mole VIII in aqueous NaOH (0.2 mole) at  $5^\circ$ , allowed to stand 1 hr., and the precipitate purified by  $C_5H_5N$ , yields almost 100% of 2-furyl-4-amino-5-phenylazo-6-hydroxypyrimidine (IX), yellow, m.  $310^\circ$ .  $Na_2S_2O_4$ , added to a suspension of IX in boiling water until the mixture is colorless, allowed to stand, and the precipitate purified by water, yields 92% of 2-furyl-4,5-diamino-6-hydroxypyrimidine (X), m.  $231^\circ$ . Prepared by the procedure used for X, the yield of  $N:CPh.N:C(OH).CH:CNH_2$ , m.  $252^\circ$ , is 60% (cf. 21% of Baddiley, et al., C.A. 37, 6667.8). Prepared analogously to IX, the yield of 2-phenyl-4-amino-5-phenylazo-6-hydroxypyrimidine, yellow (from  $C_5H_5N$ ), m.  $306^\circ$ , is 100%. Prepared analogously to X, the yield of  $N:CPh.N:C(OH).C(NH_2):CNH_2$ , m.  $228^\circ$  (from water), is 80% [cf. Traube and Herrmann, Ber. 37, 2268(1904)].

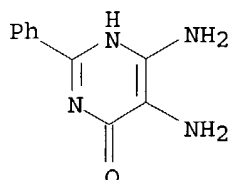
Eighteen 2-furyl- and 2-phenylpterins of the general constitution III were prepared. The following new III are reported [Ar, X, X', empirical formula, color, m.p., time of reaction (min.), reaction solvent, and solvent for purification given]: where Ar = 2-furyl (X = X'): H,  $C_{10}H_6O_2N_4$ , light yellow,  $288^\circ$ , 5, water, xylene; HO,  $C_{10}H_6O_4N_4$ , light yellow,  $330^\circ$ , 60, water, 30% AcOH; Me,  $C_{12}H_{14}O_2N_4$ , light yellow,  $266^\circ$ , 60, water, xylene; Ph,  $C_{22}H_{14}O_2N_4$ , yellow,  $281^\circ$ , 60, 50% AcOH, AcOH; p- $MeC_6H_4$ ,  $C_{24}H_{14}O_2N_4$ , yellow,  $295^\circ$ , 60, 95% AcOH, AcOH; 2-furyl,  $C_{18}H_{10}O_4N_4$ , yellow,  $268^\circ$ , 60, 50% AcOH, AcOH; 5-methyl-2-furyl,  $C_{20}H_{14}O_4N_4$ , dirty yellow,  $220^\circ$ , 60, 33% AcOH, xylene; Ar = 2-furyl: o,o'-biphenylene,  $C_{22}H_{12}O_2N_4$ , yellow,  $373^\circ$ , 30, 66%, AcOH; 1,2-acenaphthenylene,  $C_{20}H_{10}O_2N_4$ , yellow,  $358^\circ$ , 60, AcOH, AcOH; Ar = Ph (X = X'): H,  $C_{12}H_8ON_4$ , white,  $264^\circ$ , 60, water, xylene; HO,  $C_{12}H_8O_3N_4$ , white,  $370^\circ$ , 120, water, water; Me,  $C_{14}H_{12}ON_4$ , rose,  $280^\circ$ , 60, water, xylene; Ph,  $C_{24}H_{16}ON_4$ , white,  $306^\circ$ , 60, 7% AcOH, AcOH; p- $MeC_6H_4$ ,  $C_{26}H_{20}ON_4$ , light yellow,  $342^\circ$ , 60, 95% AcOH, AcOH; 2-furyl,  $C_{26}H_{12}O_3N_4$ , yellow,  $322^\circ$ , 60, 17% AcOH, AcOH; 5-methyl-2-furyl,  $C_{22}H_{16}O_3N_4$ , yellow,  $238^\circ$ , 60, 95% AcOH, EtOH; Ar = Ph: o,o'-biphenylene,  $C_{24}H_{14}ON_4$ , light yellow,  $403-4^\circ$ , 30, 15% AcOH,  $C_5H_5N$ ; 1,2-acenaphthenylene,  $C_{22}H_{12}ON_4$ , light yellow,  $388^\circ$ , 60, AcOH, AcOH.

IT 61595-45-7, 4-Pyrimidinol, 5,6-diamino-2-phenyl- (preparation of)

RN 61595-45-7 CAPLUS

CN 4(1H)-Pyrimidinone, 5,6-diamino-2-phenyl- (9CI) (CA INDEX NAME)

09/ 811,359



=> d his

(FILE 'HOME' ENTERED AT 10:41:35 ON 21 FEB 2004)

FILE 'REGISTRY' ENTERED AT 10:41:51 ON 21 FEB 2004

L1 STRUCTURE UPLOADED  
L2 STRUCTURE UPLOADED  
L3 STRUCTURE UPLOADED  
L4 8401 S L1 FUL  
L5 5166 S L2 FUL  
L6 316 S L3 FUL

FILE 'CAPLUS' ENTERED AT 10:45:05 ON 21 FEB 2004

L7 1933 S L4 OR L5  
L8 878 S L7 NOT (PYRIDYL OR PYRIDIN? OR PYRIMIDIN? OR PYRIMIDYL OR PYR  
L9 81 S L8 AND (PHENYL OR NAPHTHYL)  
L10 68 S L6  
L11 74 S L9 NOT L10

=> d l1l 1- ibib abs fhitr

'L1L' IS NOT A VALID FORMAT FOR FILE 'CAPLUS'

The following are valid formats:

ABS ----- GI and AB  
ALL ----- BIB, AB, IND, RE  
APPS ----- AI, PRAI  
BIB ----- AN, plus Bibliographic Data and PI table (default)  
CAN ----- List of CA abstract numbers without answer numbers  
CBIB ----- AN, plus Compressed Bibliographic Data  
DALL ----- ALL, delimited (end of each field identified)  
DMAX ----- MAX, delimited for post-processing  
FAM ----- AN, PI and PRAI in table, plus Patent Family data  
FBIB ----- AN, BIB, plus Patent FAM  
IND ----- Indexing data  
IPC ----- International Patent Classifications  
MAX ----- ALL, plus Patent FAM, RE  
PATS ----- PI, SO  
SAM ----- CC, SX, TI, ST, IT  
SCAN ----- CC, SX, TI, ST, IT (random display, no answer numbers;  
SCAN must be entered on the same line as the DISPLAY,  
e.g., D SCAN or DISPLAY SCAN)  
STD ----- BIB, IPC, and NCL  
  
IABS ----- ABS, indented with text labels  
IALL ----- ALL, indented with text labels  
IBIB ----- BIB, indented with text labels  
IMAX ----- MAX, indented with text labels  
ISTD ----- STD, indented with text labels  
  
OBIB ----- AN, plus Bibliographic Data (original)

09/ 811,359

OIBIB ----- OIBIB, indented with text labels

SBIB ----- BIB, no citations

SIBIB ----- IBIB, no citations

HIT ----- Fields containing hit terms

HITIND ----- IC, ICA, ICI, NCL, CC and index field (ST and IT)  
containing hit terms

HITRN ----- HIT RN and its text modification

HITSTR ----- HIT RN, its text modification, its CA index name, and  
its structure diagram

HITSEQ ----- HIT RN, its text modification, its CA index name, its  
structure diagram, plus NTE and SEQ fields

FHITSTR ----- First HIT RN, its text modification, its CA index name, and  
its structure diagram

FHITSEQ ----- First HIT RN, its text modification, its CA index name, its  
structure diagram, plus NTE and SEQ fields

KWIC ----- Hit term plus 20 words on either side

OCC ----- Number of occurrence of hit term and field in which it occurs

To display a particular field or fields, enter the display field codes. For a list of the display field codes, enter HELP DFIELDS at an arrow prompt (=>). Examples of formats include: TI; TI,AU; BIB,ST; TI,IND; TI,SO. You may specify the format fields in any order and the information will be displayed in the same order as the format specification.

All of the formats (except for SAM, SCAN, HIT, HITIND, HITRN, HITSTR, FHITSTR, HITSEQ, FHITSEQ, KWIC, and OCC) may be used with DISPLAY ACC to view a specified Accession Number.

ENTER DISPLAY FORMAT (BIB):

ENTER DISPLAY FORMAT (BIB):ibib abs fhitrn

YOU HAVE REQUESTED DATA FROM 74 ANSWERS - CONTINUE? Y/(N):y

L11 ANSWER 1 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:870461 CAPLUS

DOCUMENT NUMBER: 139:369336

TITLE: Cosmetic compositions containing tetrazoles for  
increasing hair growth and/or for preventing or hair  
loss

INVENTOR(S): Michelet, Jean-Francois; Bernard, Bruno; Rozot, Roger;  
Boulle, Christophe

PATENT ASSIGNEE(S): L'Oreal, Fr.

SOURCE: Eur. Pat. Appl., 35 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1358868	A2	20031105	EP 2003-290990	20030423
EP 1358868	A3	20031119		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
FR 2838641	A1	20031024	FR 2002-5067	20020423
PRIORITY APPLN. INFO.:				
			FR 2002-5067	A 20020423
			FR 2002-13461	A 20021028

OTHER SOURCE(S): MARPAT 139:369336

AB A cosmetic composition contains an inhibitor of 15-hydroxyprostaglandin dehydrogenase and excipient. The composition can be used to treat hair loss or act as a growth stimulant. Thus, a hair lotion contained 1-phenyl

09/ 811,359

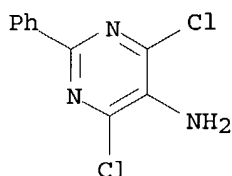
-2-(2-phenyl-2H-tetrazol-5-yl)ethanone 0.80, propylene glycol 10.00, and isopropanol qs to 100 g. The composition decreased the hair loss and stimulated hair growth.

IT 20959-02-8

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)  
(cosmetic compns. containing tetrazoles for increasing hair growth and/or for preventing or hair loss)

RN 20959-02-8 CAPLUS

CN 5-Pyrimidinamine, 4,6-dichloro-2-phenyl- (9CI) (CA INDEX NAME)



L11 ANSWER 2 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:837577 CAPLUS

DOCUMENT NUMBER: 139:341428

TITLE: Hair cosmetic compositions to support the growth and/or delay the fall of hair

INVENTOR(S): Michelet, Jean Francois; Bernard, Bruno

PATENT ASSIGNEE(S): L'Oreal, Fr.

SOURCE: Fr. Demande, 34 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent

LANGUAGE: French

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
FR 2838641	A1	20031024	FR 2002-5067	20020423
EP 1358868	A2	20031105	EP 2003-290990	20030423
EP 1358868	A3	20031119		

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK

WO 2003090699	A1	20031106	WO 2003-FR1285	20030423
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W: CA, JP, US

PRIORITY APPLN. INFO.: FR 2002-5067 A 20020423

FR 2002-13461 A 20021028

AB The invention relates to a cosmetic composition containing an inhibitor of the 15-hydroxyprostaglandin dehydrogenase and cosmetic excipients. It also relates to a process of treatment to support the growth and/or to prevent or delay the fall of the hair, as well as the use of an inhibitor of 15-hydroxyprostaglandin dehydrogenase. Thus, 2-phenyl-4,6-dichloro-5-aminopyrimidine inhibited the 15-hydroxyprostaglandin dehydrogenase by 43%.

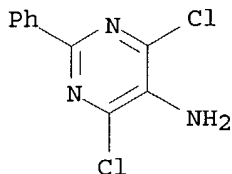
IT 20959-02-8

RL: COS (Cosmetic use); BIOL (Biological study); USES (Uses)  
(hair cosmetic compns. for delaying fall of hair)

RN 20959-02-8 CAPLUS

CN 5-Pyrimidinamine, 4,6-dichloro-2-phenyl- (9CI) (CA INDEX NAME)

09/ 811,359



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 3 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:804504 CAPLUS

DOCUMENT NUMBER: 140:59596

TITLE: New N6- or N(9)-hydroxyalkyl substituted 8-azaadenines or adenines as effective A1 adenosine receptor ligands  
AUTHOR(S): Biagi, Giuliana; Giorgi, Irene; Leonardi, Michele; Livi, Oreste; Pacchini, Federica; Scartoni, Valerio; Costa, Barbara; Lucacchini, Antonio

CORPORATE SOURCE: Dipartimento di Scienze Farmaceutiche, Universita di Pisa, Pisa, I-56126, Italy

SOURCE: European Journal of Medicinal Chemistry (2003), 38(9), 801-810

CODEN: EJMCA5; ISSN: 0223-5234

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB In this paper the authors describe synthesis and biol. assays of some A1 ligands more water-soluble than the effective, but very lipophilic, 8-azaadenines and adenines discovered in the past and obtained introducing on N6 or N(9) substituent a hydroxy group. Five of the new N6-hydroxyalkyl- and N6-hydroxycycloalkyl-2-phenyl-9-benzyl-8-azaadenines showed very high affinity ( $K_i < 40$  nM) and selectivity for A1 adenosine receptors. Among the 2-phenyl-9-(2-hydroxy-3-alkyl)-8-azaadenines or adenines prepared, the compds. with the higher A1 affinity and selectivity were 2-phenyl-9-(2-hydroxy-3-propyl)-N6-cyclopentyl- and cyclohexyl-8-azaadenine with  $K_i 2.2 \pm 0.2$  nM and  $2.8 \pm 0.3$  nM resp. From the point of view of water-solubility, 2-phenyl-9-(2-hydroxy-3-propyl)-8-azaadenine was the most interesting compound, having a CLogP of 1.066991 and a water-solubility of 1.2 mg mL<sup>-1</sup>.

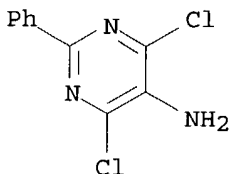
IT 20959-02-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of N6- or N(9)-hydroxyalkyl substituted 8-azaadenines or adenines as effective water-soluble A1 adenosine receptor ligands)

RN 20959-02-8 CAPLUS

CN 5-Pyrimidinamine, 4,6-dichloro-2-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 4 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:376819 CAPLUS



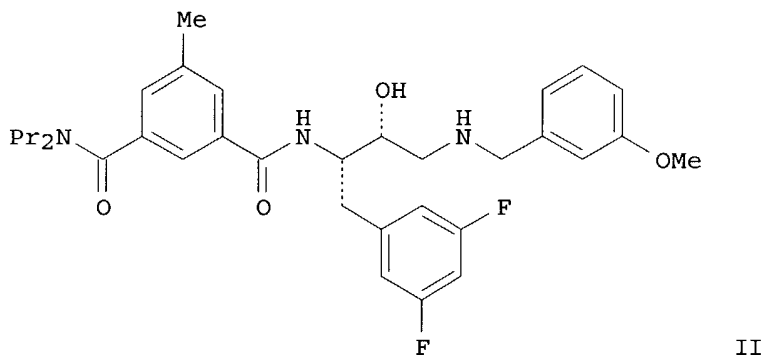
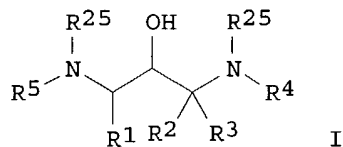
09/ 811,359

DOCUMENT NUMBER: 138:385173  
TITLE: Preparation of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease  
INVENTOR(S): Varghese, John; Maillard, Michel; Jagodzinska, Barbara; Beck, James P.; Gailunas, Andrea; Fang, Larry; Sealy, Jennifer; Tenbrink, Ruth; Freskos, John; Mickelson, John; Samala, Lakshman; Hom, Roy  
PATENT ASSIGNEE(S): Elan Pharmaceuticals, Inc., USA; Pharmacia & Upjohn Company  
SOURCE: PCT Int. Appl., 1243 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003040096	A2	20030515	WO 2002-US36072	20021108
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			
WO 2003040096	A2	20030515	WO 2002-XA36072	20021108
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG			

PRIORITY APPLN. INFO.:  
US 2001-337122P P 20011108  
US 2001-344086P P 20011228  
US 2002-345635P P 20020103  
WO 2002-US36072 A 20021108

OTHER SOURCE(S): MARPAT 138:385173  
GI



AB The title compds. [I; R1 = (un)substituted alkyl, alkenyl, alkynyl, etc.; R2 = H, alkyl, haloalkyl, alkenyl, etc.; R3 = H, alkyl, haloalkyl, alkenyl, etc.; or R2 and R3 are taken together with the carbon to which they are attached to form a carbocycle of 3-7 carbon atoms, optionally where one carbon atom is replaced by a heteroatom selected from the group consisting of O, S, SO2, (un)substituted NH; R4 = alkyl, haloalkyl, hydroxyalkyl, etc.; R5 = R6X (wherein X = CO, SO2, (un)substituted CH2; R6 = (un)substituted Ph, **naphthyl**, indanyl, etc.); R25 = H, alkyl, alkoxy, etc.] which have activity as inhibitors of  $\beta$ -secretase and are therefore useful in treating a variety of disorders such as Alzheimer's disease, were prepared. E.g., a multi-step synthesis of (1S,2R)-II, starting from (2S)-2-[(tert-butoxycarbonyl)amino]-3-(3,5-difluorophenyl)propanoic acid, was given. The compds. I showed IC50 of < 20  $\mu$ M in cell free inhibition assay utilizing a synthetic APP substrate. This is a Part 1 of 1-2 series.

IT 527729-81-3P

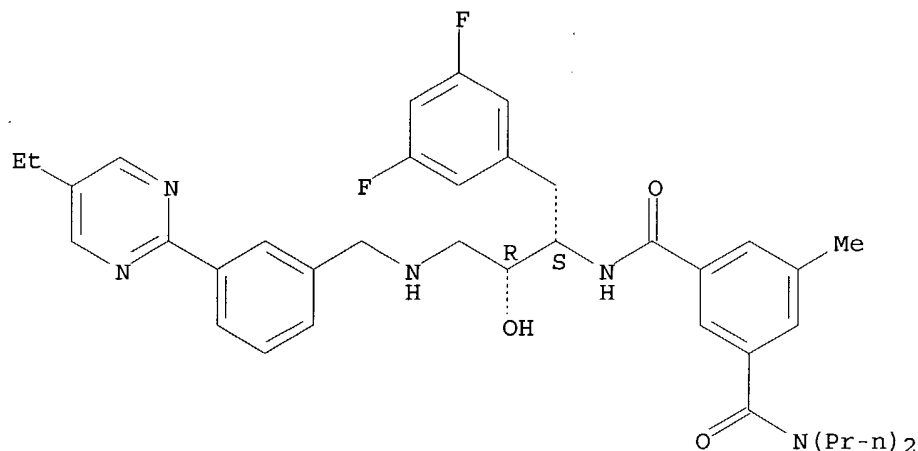
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N,N'-substituted-1,3-diamino-2-hydroxypropanes for treating Alzheimer's disease)

RN 527729-81-3 CAPLUS

CN 1,3-Benzenedicarboxamide, N'-[(1S,2R)-1-[(3,5-difluorophenyl)methyl]-3-[[[3-(5-ethyl-2-pyrimidinyl)phenyl]methyl]amino]-2-hydroxypropyl]-5-methyl-N,N-dipropyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 5 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2003:96444 CAPLUS

DOCUMENT NUMBER: 138:329338

TITLE: A novel frustrated phase produced by a binary system of nonsymmetric dimeric liquid crystals

AUTHOR(S): Yoshizawa, Atsushi; Yamamoto, Kazuyuki; Dewa, Harutada; Nishiyama, Isa; Yamamoto, Jun; Yokoyama, Hiroshi

CORPORATE SOURCE: Department of Materials Science and Technology, Faculty of Science and Technology, Hirosaki University, Hirosaki, 036-8561, Japan

SOURCE: Journal of Materials Chemistry (2003), 13(2), 172-174  
CODEN: JMACEP; ISSN: 0959-9428

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

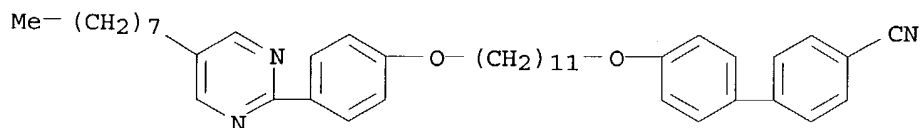
AB A novel frustrated liquid-crystalline phase was obtained in some binary mixts. between polar nonsym. dimeric liquid crystals,  $\alpha$ -(4-cyanobiphenyl-4'-yloxy)- $\omega$ -[4-(5-alkylpyrimidin-2-yl) phenyl-4''-oxy]alkanes; it appeared below nematic or smectic A phases and was found not to possess a clear layered structure.

IT 213549-33-8

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)  
(frustrated phase in binary system of (cyanobiphenylyloxy)[(alkylpyrimidinyl)phenyloxy]alkane liquid crystals)

RN 213549-33-8 CAPLUS

CN [1,1'-Biphenyl]-4-carbonitrile, 4'-[[11-[4-(5-octyl-2-pyrimidinyl)phenoxy]undecyl]oxy]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

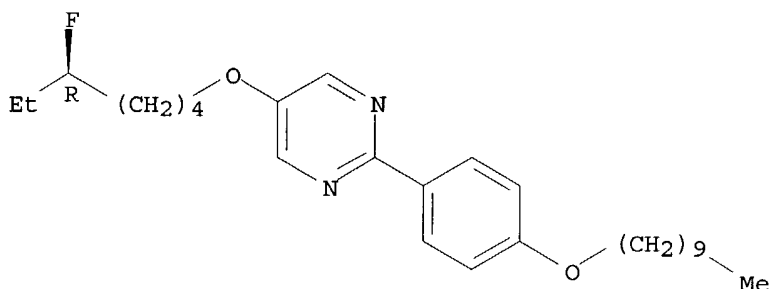
L11 ANSWER 6 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:790550 CAPLUS

09/ 811,359

DOCUMENT NUMBER: 138:100099  
TITLE: Optical resolution of 5-alkyl- $\delta$ -valerolactones and synthesis of optically active 5-fluoroalkanols  
AUTHOR(S): Riswoko, Asep; Aoki, Yoshio; Hirose, Takuji; Nohira, Hiroyuki  
CORPORATE SOURCE: Department of Applied Chemistry, Faculty of Engineering, Saitama University, Urawa, 338-8570, Japan  
SOURCE: Enantiomer (2002), 7(1), 33-39  
CODEN: EANTE2; ISSN: 1024-2430  
PUBLISHER: Taylor & Francis Ltd.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Optical resolsns. of 5-alkyl- $\delta$ -valerolactones were carried out by derivatization to the diastereomeric amides, in which (R)-(+)-1-(1-naphthyl)ethylamine or (S)-(-)-1-phenylethylamine were used as resolving agents. Optically active 5-fluoroalkanols, useful intermediates for fluorinated ferroelec. liquid crystals, were derived from the resolved lactones in four steps without racemization.  
IT 483287-73-6P  
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and properties of)  
RN 483287-73-6 CAPLUS  
CN Pyrimidine, 2-[4-(decyloxy)phenyl]-5-[[[(5R)-5-fluoroheptyl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

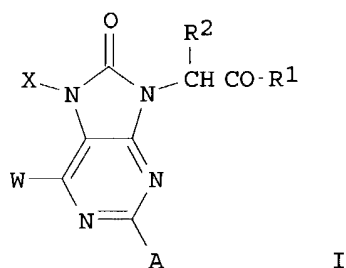


REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

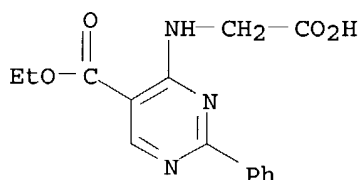
L11 ANSWER 7 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2002:439079 CAPLUS  
DOCUMENT NUMBER: 137:6192  
TITLE: Preparation of 2-(7,8-dihydro-8-oxo-9H-purin-9-yl)acetic acids  
INVENTOR(S): Masumoto, Kaoru; Murata, Akiya  
PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 18 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002167387	A2	20020611	JP 2000-362126	20001129
PRIORITY APPLN. INFO.:			JP 2000-362126	20001129
OTHER SOURCE(S):		MARPAT 137:6192		

GI



- AB Title compds. I [R1 = OH, NH2, NHR3; R3 = lower alkyl, alkenyl, cycloalkyl, benzyloxy, etc.; R2 = H, lower alkyl, hydroxyalkyl, (un)substituted benzyloxyalkyl; W = H, lower alkyl, halo, lower alkoxy, NH2, etc.; X = H, lower alkyl, cycloalkylalkyl, phenylalkyl, alkenyl, alkanoyl, etc.; A = (un)substituted Ph, heteroaryl] or their salts are prepared. The compds. are useful as materials for anxiety inhibitors, antidepressants, and antiepileptics. 2-(7,8-Dihydro-8-oxo-2-phenyl-9H-purin-9-yl)acetonitrile (2.5 g) was treated with NaOH in EtOH at 80° for 2 h to give 1.5 g 2-(7,8-dihydro-8-oxo-2-phenyl-9H-purin-9-yl)acetic acid.
- IT **226954-91-2**, 2-[(5-Ethoxycarbonyl-2-phenylpyrimidin-4-yl)amino]acetic acid  
 RL: RCT (Reactant); RACT (Reactant or reagent)  
 (preparation of (dihydrooxopurinyl)acetic acid)
- RN **226954-91-2** CAPLUS
- CN 5-Pyrimidinecarboxylic acid, 4-[(carboxymethyl)amino]-2-phenyl-, 5-ethyl ester (9CI) (CA INDEX NAME)



- L11 ANSWER 8 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN
- ACCESSION NUMBER: 2002:261297 CAPLUS
- DOCUMENT NUMBER: 137:13584
- TITLE: Layer compression modulus in smectic liquid crystals
- AUTHOR(S): Shibahara, Seiji; Yamamoto, Jun; Takanishi, Yoichi; Ishikawa, Ken; Takezoe, Hideo
- CORPORATE SOURCE: Department of Organic and Polymeric Materials, Tokyo Institute of Technology, Tokyo, 152-8552, Japan
- SOURCE: Journal of the Physical Society of Japan (2002), 71(3), 802-807  
 CODEN: JUPSAU; ISSN: 0031-9015
- PUBLISHER: Physical Society of Japan
- DOCUMENT TYPE: Journal
- LANGUAGE: English
- AB The layer compression modulus B for smectic liquid crystals near the SmA-SmC\*, SmA-SmC\*A, SmA-ferrielec. phase transitions. B shows a significant pretransitional softening due to the order parameter fluctuations above the phase transitions, suggesting that these phase transitions are not of the Landau mean-field type. B was also measured

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near the nematic-SmA and SmA-CryB phase transitions. In the vicinity of the nematic-SmA phase transition, critical exponent of B is in very good agreement with that determined by light scattering. At the SmA-CryB phase transition, B suddenly increases without pretransitional behavior.

IT 129409-27-4

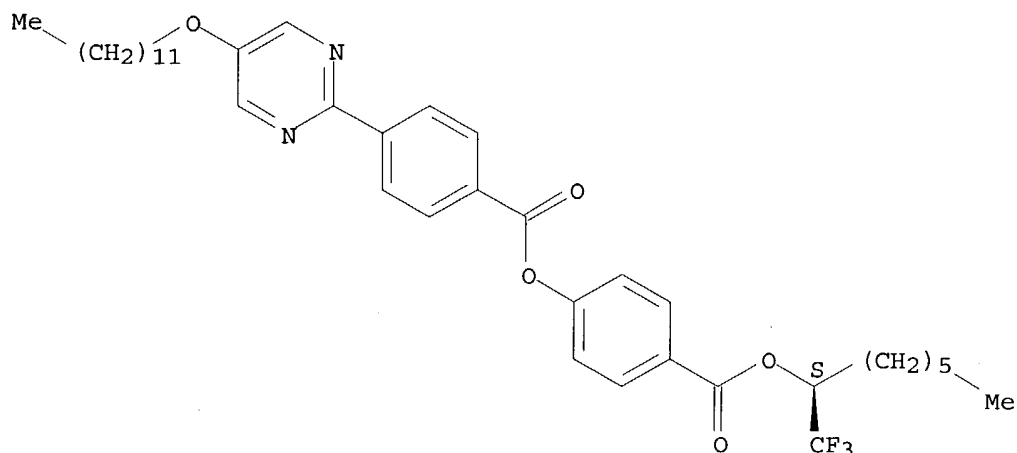
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PYP (Physical process); PROC (Process)

(layer compression modulus in smectic liquid crystals near phase transitions)

RN 129409-27-4 CAPLUS

CN Benzoic acid, 4-[5-(dodecyloxy)-2-pyrimidinyl]-, 4-[[[(1S)-1-(trifluoromethyl)heptyl]oxy]carbonyl]phenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 9 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:235346 CAPLUS

DOCUMENT NUMBER: 138:32776

TITLE: erythro- and threo-2-Hydroxynonyl substituted 2-phenyladenines and 2-phenyl-8-azaadenines: ligands for A1 adenosine receptors and adenosine deaminase

AUTHOR(S): Biagi, Giuliana; Giorgi, Irene; Livi, Oreste; Pacchini, Federica; Rum, Pietro; Scartoni, Valerio; Costa, Barbara; Mazzoni, Maria Rosa; Giusti, Laura  
CORPORATE SOURCE: Department of Pharmaceutical Sciences, University of Pisa, Pisa, 56126, Italy

SOURCE: Farmaco (2002), 57(3), 221-233  
CODEN: FRMCE8; ISSN: 0014-827X

PUBLISHER: Editions Scientifiques et Medicales Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Erythro-2-Phenyl-9-(2-hydroxy-3-nonyl)adenine and its 8-aza analog were prepared and showed a very high inhibitory activity towards adenosine deaminase (ADA), with Ki 0.55 and 1.67 nM, resp., and high affinity for A1 adenosine receptors, with Ki 28 and 2.8 nM, resp. To increase affinity for A1 receptors we introduced a substituent on the N6 position such as alkyl or cycloalkyl groups, which are present in effective agonists or antagonists. Furthermore, for some compds., we prepared the two diastereoisomers erythro and threo to verify whether the binding with A1 receptors is stereoselective, as in ADA. Results show that some of the synthesized compds. are good inhibitors for ADA and good

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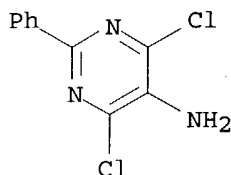
ligands for A1, and the erythro diastereoisomers are more active than the threo ones. The exptl. evidence allows us to hypothesize some similarity in the three dimensional structures of the binding site of the two proteins, ADA and A1 adenosine receptor, in spite of lacking any homologies in the amino acid sequences.

IT 20959-02-8

RL: RCT (Reactant); RACT (Reactant or reagent)  
(phenyladenines and phenylazaadenines as ligands for A1 adenosine receptors and adenosine deaminase inhibitors)

RN 20959-02-8 CAPLUS

CN 5-Pyrimidinamine, 4,6-dichloro-2-phenyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 10 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2002:177700 CAPLUS

DOCUMENT NUMBER: 136:195461

TITLE: Structure-activity relationships for gene activation oestrogenicity: evaluation of a diverse set of aromatic chemicals

AUTHOR(S): Schultz, T. Wayne; Sink, Glendon D.; Cronin, Mark T. D.

CORPORATE SOURCE: Department of Comparative Medicine, College of Veterinary Medicine, The University of Tennessee, Knoxville, TN, 37996-4500, USA

SOURCE: Environmental Toxicology (2002), 17(1), 14-23  
CODEN: ETOXFH; ISSN: 1520-4081

PUBLISHER: John Wiley & Sons, Inc.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Structure-activity relationships for estrogenicity were developed based on 120 aromatic chems. evaluated in the *Saccharomyces cerevisiae*-based Lac-Z reporter assay. Relative gene activation was compared to 17 $\beta$ -estradiol and varied over eight orders of magnitude. Anal. of the data compared to 17 $\beta$ -estradiol identified three structural criteria that were related to xenoestrogen activity and potency: (1) the hydrogen-bonding ability of the phenolic ring mimicking the A-ring, (2) a hydrophobic center similar in size and shape to the B- and C-rings, and (3) a hydrogen-bond donor mimicking the 17 $\beta$ -hydroxyl moiety of the D-ring, especially with an oxygen-to-oxygen distance similar to that between the 3- and 17 $\beta$ -hydroxyl groups of 17 $\beta$ -estradiol. Binding data were segregated into activity clusters including strong, moderate, weak, and detectable gene expression, and those compds. that were inactive. The hydrogen-bonding ability of hydroxy group in the 3-position on 17 $\beta$ -estradiol was observed to be essential for gene activation. Compds. with a 4-hydroxyl substituted benzene ring and a hydrophobic moiety of size and shape equivalent to the B-ring of 17 $\beta$ -estradiol were generally observed to be weakly active compds. Moderately active compds. have a 4-hydroxyl substituted benzene ring with a hydrophobic moiety equivalent in size and shape to the B- and C-ring of 17 $\beta$ -estradiol, or have a high hydrogen-bond donor capacity owing to the presence of halogens on a nonphenolic ring. Strongly active compds., similar to 4,4'-diethylethylene bisphenol (DES), possess the same hydrophobic ring

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structure as described for moderately active compds. and an addnl. hydroxyl group with an oxygen-to-oxygen distance close to that exhibited by the 3- and 17-hydroxyl groups of 17 $\beta$ -estradiol.

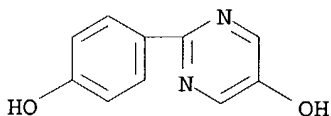
IT 142172-97-2

RL: ADV (Adverse effect, including toxicity); PRP (Properties); BIOL (Biological study)

(structure-activity relationships of diverse set of aromatic chems. for gene activation estrogenicity)

RN 142172-97-2 CAPLUS

CN 5-Pyrimidinol, 2-(4-hydroxyphenyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 11 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:767018 CAPLUS  
Correction of: 1996:672852

DOCUMENT NUMBER: 135:273074  
Correction of: 126:31466

TITLE: Boronic acid and ester inhibitors of thrombin  
INVENTOR(S): Amparo, Eugene C.; Miller, William H.; Pacofsky, Gregory J.; Wityak, John; Weber, Patricia C.; Duncia, John J. V.; Santella, Joseph B., III

PATENT ASSIGNEE(S): The DuPont Merck Pharmaceutical Company, USA

SOURCE: U.S., 170 pp., Cont.-in-part of U.S. Ser. No. 348,029.  
CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 3

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5563127	A	19961008	US 1994-364338	19941227
CA 2208971	AA	19960711	CA 1995-2208971	19951213
CA 2208971	C	20010116		
WO 9620689	A2	19960711	WO 1995-US16248	19951213
WO 9620689	A3	19961024		
W: AU, CA, JP, MX, NZ				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
AU 9646404	A1	19960724	AU 1996-46404	19951213
EP 810858	A2	19971210	EP 1995-944331	19951213
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
ZA 9510978	A	19970627	ZA 1995-10978	19951227
US 5698538	A	19971216	US 1996-690220	19960726

PRIORITY APPLN. INFO.:  
US 1993-36377 B2 19930324  
US 1994-318029 B2 19941004  
US 1994-348029 A2 19941201  
US 1994-364338 A 19941227  
WO 1995-US16248 W 19951213

AB Novel boronic acid and ester and carboxyl-modified amino acid compds. R1-Z-CHR2-A (A = organoboryl, BY1Y2; Y1, Y2 = independently OH, F, organoamino, C1-8 alkoxy, Y1Y2 = cyclic boron ester, amide containing N, S, O; etc.; Z = (CH2)mCX, X = amido, thioamido, etc., substituted C1-12 alkyl, alkenyl, etc.; R1 = arylalkenyl, aryl = substituted Ph, **naphthyl**, biphenyl, etc.; R2 = substituted C1-12 alkyl, alkenyl, etc.), which are



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inhibitors of trypsin-like enzymes, are disclosed. Thus, amino acid modified boronic ester (Y1Y2 = (+)-pinanediol) was prepared in multiple steps starting from (+)-pinanediol 4-bromo-1(R)-(4-phenylbenzoyl)aminobutane-1-boronate. Thrombin inhibition activity of some of the compds. prepared is described.

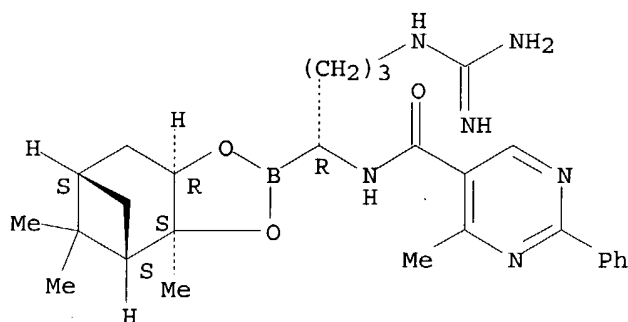
IT 180896-93-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of amino acid-modified boronic acids and esters as inhibitors of thrombin)

RN 180896-93-9 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[(1R)-4-[(aminoiminomethyl)amino]-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]butyl]-4-methyl-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 12 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:372157 CAPLUS

DOCUMENT NUMBER: 134:366894

TITLE: Preparation of 2-(4-trifluoromethylphenyl)-4-aminopyrimidines as remedies for autoimmune inflammatory diseases

INVENTOR(S): Murata, Akiya; Kondo, Masanori; Ohno, Kazunori; Tanaka, Masayasu; Ito, Masato

PATENT ASSIGNEE(S): Dainippon Pharmaceutical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

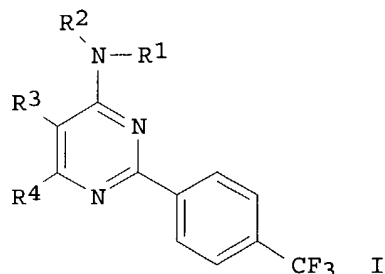
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001139560	A2	20010522	JP 1999-326299	19991117
PRIORITY APPLN. INFO.:			JP 1999-326299	19991117
OTHER SOURCE(S):		MARPAT 134:366894		

GI



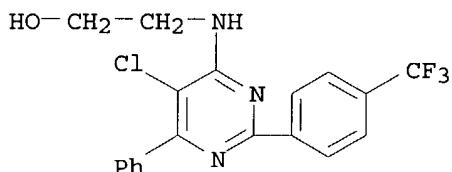
AB The title compds. I [R1 = H, alkyl, etc.; R2 = alkyl, etc.; further detail on R1 and R2 is given; R3 = halo, etc.; R4 = alkyl, (un)substituted Ph, etc.] are prepared I [NR1R2 = NHCH2CH(OH)Me; R3 = Cl; R4 = **phenyl**] at 3 mg/kg/day orally (5 days/wk; for 7.4 wk) gave 98.2 % inhibition of collagen-induced arthritis in mice. Formulations are given.

IT **340149-33-9P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of aminopyrimidines as remedies for autoimmune inflammatory diseases)

RN 340149-33-9 CAPLUS

CN Ethanol, 2-[[5-chloro-6-phenyl-2-[4-(trifluoromethyl)phenyl]-4-pyrimidinyl]amino]- (9CI) (CA INDEX NAME)



L11 ANSWER 13 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:238802 CAPLUS

DOCUMENT NUMBER: 135:12839

TITLE: Ferroelectric Liquid Crystals Induced by Atropisomeric Biphenyl Dopants: Dependence of the Polarization Power on the Nature of the Symmetry-Breaking Groups

AUTHOR(S): Vizitiu, Despina; Lazar, Carmen; Radke, Joshua P.; Hartley, C. Scott; Glaser, Matthew A.; Lemieux, Robert P.

CORPORATE SOURCE: Department of Chemistry, Queen's University, Kingston, ON, K7L 3N6, Can.

SOURCE: Chemistry of Materials (2001), 13(5), 1692-1699  
CODEN: CMATEX; ISSN: 0897-4756

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Four new chiral dopants containing an atropisomeric biphenyl core derived from 4,4'-dihydroxy-2,2',6,6'-tetramethylbiphenyl with different symmetry-breaking groups at the 3,3'-positions (X = F, Cl, Br, and Me) were synthesized in optically active form. These dopants were used to induce ferroelec. SmC\* liquid crystal phases in four SmC hosts with different core structures. Polarization powers  $\delta p$  were measured as a function of the SmC host and compared to  $\delta p$  values previously obtained for an analogous atropisomeric dopant with X = NO2. Theor.

conformational analyses for rotation of the atropisomeric cores about the C-O bonds of the ester groups linking the core to the side chains were performed at the B3LYP/6-31G(d) level and used in calculating Boltzmann-weighted statistical average transverse dipole moments  $\langle \mu_{\perp} \rangle$  for the core-diester units. The  $\langle \mu_{\perp} \rangle$  values were used to normalize  $\delta p$  to study the influence of the symmetry-breaking groups X on the polar ordering of the dopants. Variations in  $\delta p(\text{norm})$  are rationalized by considering models describing either achiral or chiral distortions of the zigzag binding site model of the SmC host. The symmetry-breaking groups X exert a unique influence on polar ordering of the dopants in the phenylpyrimidine host PhP1 that is consistent with a model in which chirality transfer via core-core interactions between dopant and host mols. causes a chiral distortion of the zigzag binding site.

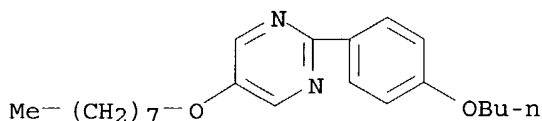
IT 121083-89-4

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(ferroelec. Liquid Crystals Induced by Atropisomeric Biphenyl Dopants: Dependence of Polarization Power on Nature of Symmetry-Breaking Groups)

RN 121083-89-4 CAPLUS

CN Pyrimidine, 2-(4-butoxyphenyl)-5-(octyloxy)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 14 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:235545 CAPLUS

DOCUMENT NUMBER: 134:273626

TITLE: Optically active compound, ferroelectric/antiferroelectric liquid crystal composition, and liquid crystal device using it

INVENTOR(S): Takiguchi, Takao; Hanyu, Yukio; Sato, Koichi; Nakamura, Shinichi; Noguchi, Koji; Shimizu, Yasushi

PATENT ASSIGNEE(S): Canon Inc., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 22 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001089421	A2	20010403	JP 1999-267903	19990922
PRIORITY APPLN. INFO.:			JP 1999-267903	19990922

OTHER SOURCE(S): MARPAT 134:273626

AB The compound comprises RA1X1A2(X2A3)mX3CH(CF3)CH2O(CH2)nB [R = C1-20 alkyl; A1-A3 = (substituted) divalent cyclic group; m = 0, 1; n = 2-20; X1, X2 = none, CO<sub>2</sub>, O<sub>2</sub>C, CH<sub>2</sub>O, OCH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>, CH:CH; C.tplbond.C; X3 = CO<sub>2</sub>, CH<sub>2</sub>O, O; B = (substituted) Ph, (substituted) cyclohexyl]. The liquid crystal composition contains the above compound. The liquid crystal device comprises the above composition sandwiched between a pair of substrate and a driving electrode. The display shows high response and gives high-contrast images.

IT 108572-55-0D, mixture containing

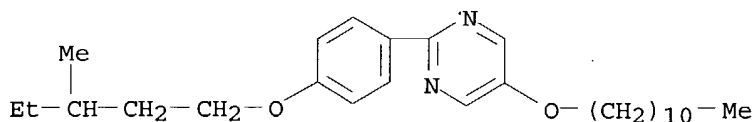
RL: DEV (Device component use); USES (Uses)

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(optically active compound for ferroelec./antiferroelec. liquid crystal composition used in display)

RN 108572-55-0 CAPLUS

CN Pyrimidine, 2-[4-[(3-methylpentyl)oxy]phenyl]-5-(undecyloxy)- (9CI) (CA INDEX NAME)



L11 ANSWER 15 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:149472 CAPLUS

DOCUMENT NUMBER: 134:340556

TITLE: Ortho-metalated complexes of 2,6-diphenylpyrimidin-4-one

AUTHOR(S): Krylova, L. F.; Terskikh, V. V.

CORPORATE SOURCE: Novosib. Gos. Univ., Russia

SOURCE: Zhurnal Neorganicheskoi Khimii (2000), 45(10), 1714-1720

CODEN: ZNOKAQ; ISSN: 0044-457X

PUBLISHER: MAIK Nauka/Interperiodica Publishing

DOCUMENT TYPE: Journal

LANGUAGE: Russian

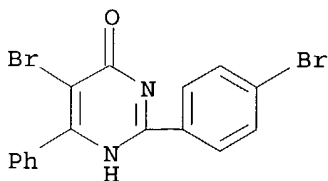
AB Title complexes of Pd(II) and Pt(II) with 2,6-diphenylpyrimidin-4-one (LH2), namely, [Pd(LH)Cl] and [M(L)en] (M = Pt, Pd; en = ethylenediamine), and also the brominated compound 2-(o-bromophenyl)-6-phenyl-5-bromopyrimidine-4-one (LBr2) were prepared. The o-palladated complex [Pd(LH)Cl] was used as selective reagent. Bromination of [Pd(LH)Cl] under stringent conditions gave LBr2. The structures of the compds. obtained were examined by 1- and 2-dimensional (homo- and heteronuclear) 1H and 13C NMR.

IT 338734-67-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 338734-67-1 CAPLUS

CN 4(1H)-Pyrimidinone, 5-bromo-2-(4-bromophenyl)-6-phenyl- (9CI) (CA INDEX NAME)



L11 ANSWER 16 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2001:77904 CAPLUS

DOCUMENT NUMBER: 134:280461

TITLE: Gas-phase pyrolysis of 2-heteroaromatic-1-dimethylaminoethylenes: kinetic and mechanistic study

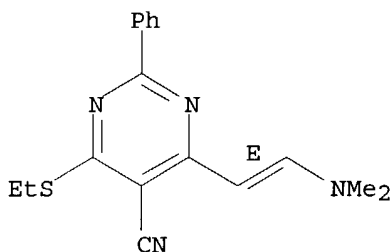
AUTHOR(S): Elnagdi, Mohamed H.; Al-Awadi, Nouria A.; Kumar, Agith; Khalik, Mervat Abdul

CORPORATE SOURCE: Chemistry Department, Kuwait University, Safat, 13060, Kuwait

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SOURCE: Heteroatom Chemistry (2001), 12(1), 47-51  
CODEN: HETCE8; ISSN: 1042-7163  
PUBLISHER: John Wiley & Sons, Inc.  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 134:280461  
AB Gas-phase pyrolysis reactions of 4(2'-dimethylaminoethenyl)-2-oxo-2H-benzo[b]pyran-3-carbonitrile (1), 4(2'-dimethylaminoethenyl)-2-oxo-2H-naphtho[1,2-b]pyran-3-carbonitrile (2), 1,6-dihydro-4-(2'-dimethylaminoethenyl)-6-oxo-1-phenylpyridazine-3,5-dicarbonitrile (3), 2-cyano-5-dimethylamino-3-phenyl-2,4-pentadienonitrile (4), 2-cyano-5-dimethylamino-3-(2-thienyl)-2,4-pentadienonitrile (5), 1,2-dihydro-4-(2'-dimethylaminoethenyl)-oxo-quinoline-4-carbonitrile (6), 6-(ethylthio)-4-(2'-dimethylaminoethenyl)-2-phenylpyrimidine-5-carbonitrile (7) have been carried out. The rates of gas-phase pyrolytic reactions of compds. 3, 4, 5, and 7 have been measured and found to correspond to unimol. first-order reactions. Product analyses together with kinetic data were used to outline a feasible pathway for the pyrolytic reactions of the compds. under study.  
IT 333722-73-9P  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)  
(gas-phase pyrolysis of 2-heteroarom.-1-dimethylaminoethylenes)  
RN 333722-73-9 CAPLUS  
CN 5-Pyrimidinecarbonitrile, 4-[(1E)-2-(dimethylamino)ethenyl]-6-(ethylthio)-2-phenyl- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 17 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 2000:441378 CAPLUS  
DOCUMENT NUMBER: 133:81642  
TITLE: Liquid crystal compound incorporating furan ring for electrooptical display device  
INVENTOR(S): Bernhardt, Henry; Kato, Takashi; Fujita, Atsuko; Takeuchi, Hiroyuki; Takeshita, Fusayuki; Nakagawa, Etsuo  
PATENT ASSIGNEE(S): Chisso Corporation, Japan  
SOURCE: Eur. Pat. Appl., 82 pp.  
CODEN: EPXXDW  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1013649	A1	20000628	EP 1999-125327	19991220

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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO

JP 2000191653 A2 20000711 JP 1999-364177 19991222  
PRIORITY APPLN. INFO.: US 1998-113506P P 19981222

OTHER SOURCE(S): MARPAT 133:81642

AB The present invention provides a liquid crystal compound incorporating a furan ring having phys. properties suitable for use in an electrooptical display device. The liquid crystal compound may be 5-(4'-trans-pentyl-trans-bicyclohexyl-4-yl)-2-methylfuran, 5-(4-(4-trans-pentylcyclohexyl)phenyl)-2-ethylfuran, 5-(trans-4-propylcyclohexyl)furan-2-yl-3,4-dibromobenzene, 2-(4-trans-pentylcyclohexyl)-5-(4-trans-propylcyclohexyl)furan, or 2-(4-trans-(2,3-difluoro-4-methoxyphenyl)cyclohexyl)-5-(5-trans-propyl-1,3-dioxan-2-yl)furan.

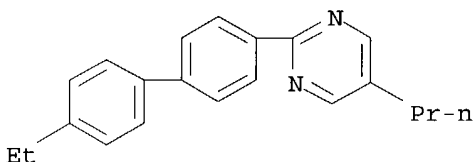
IT 175859-31-1

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(electrooptical display devices with liquid crystal compns. containing)

RN 175859-31-1 CAPLUS

CN Pyrimidine, 2-(4'-ethyl[1,1'-biphenyl]-4-yl)-5-propyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 18 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:335409 CAPLUS

DOCUMENT NUMBER: 132:334474

TITLE: Preparation of spiroindolines as Y5 receptor antagonists

INVENTOR(S): Gao, Ying-duo; Macneil, Douglas J.; Yang, Lihu; Morin, Nancy R.; Fukami, Takehiro; Kanatani, Akio; Fukuroda, Takahiro; Ishii, Yasuyuki; Morin, Masaki

PATENT ASSIGNEE(S): Merck & Co., Inc., USA; Banyu Pharmaceutical Co., Ltd.; et al.

SOURCE: PCT Int. Appl., 130 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

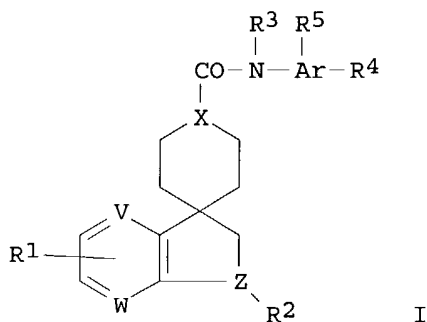
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000027845	A1	20000518	WO 1999-US26447	19991108
W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
US 6191160	B1	20010220	US 1999-436120	19991108

09/ 811,359

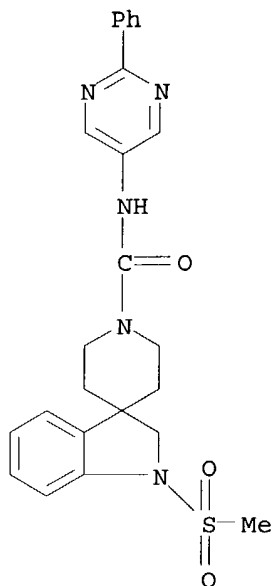
EP 1129089            A1    20010905            EP 1999-971808    19991108  
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,  
IE, SI, LT, LV, FI, RO  
AU 756797            B2    20030123            AU 2000-14732       19991108  
US 6313298           B1    20011106            US 2000-656698     20000907  
US 2002058813       A1    20020516            US 2001-896940     20010629  
US 6495559           B2    20021217  
US 6638942           B1    20031028            US 2002-228250     20020826  
PRIORITY APPLN. INFO.:            US 1998-107835P    P    19981110  
   US 1999-436120    A3   19991108  
   WO 1999-US26447    W    19991108  
   US 2000-656698    A3   20000907  
   US 2001-896940    A3   20010629

OTHER SOURCE(S):            MARPAT 132:334474  
GI



AB The title compds. I [V, W, X, Z = CH, N; R1 = H, alkyl, etc.; R2 = CHO, etc.; R3 = H, alkyl; Ar = aryl, heteroaryl; R4, R5 = H, nitro, etc.] are prepared I are useful in the treatment of obesity and the complications associated therewith. 1-Methanesulfonyl-N-(5-phenyl-2-pyrazinyl)spiro[indoline-3,4'-piperidine]-1'-carboxamide at 3 mg/kg suppressed bovine pancreatic polypeptide-induced food intake in rats. Formulations are given.

IT **268537-04-8P**  
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of spiroindolines as Y5 receptor antagonists)  
RN 268537-04-8 CAPLUS  
CN Spiro[3H-indole-3,4'-piperidine]-1'-carboxamide, 1,2-dihydro-1-(methylsulfonyl)-N-(2-phenyl-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 19 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 2000:243702 CAPLUS

DOCUMENT NUMBER: 133:17225

TITLE: Nickel- and palladium-catalyzed cross-coupling reactions at the bridgehead of bicyclo[1.1.1]pentane derivatives - a convenient access to liquid crystalline compounds containing bicyclo[1.1.1]pentane moieties

AUTHOR(S): Messner, Matthias; Kozhushkov, Sergei I.; De Meijere, Armin

CORPORATE SOURCE: Institut fur Organische Chemie der George-August-Universitat Gottingen, Gottingen, 37077, Germany

SOURCE: European Journal of Organic Chemistry (2000), (7), 1137-1155

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 133:17225

AB Radical addition reactions of organyl iodides onto [1.1.1]propellane (I) followed by halogen-lithium exchange and transmetalation with zinc chloride, as well as addns. of Grignard reagents to I, have furnished a variety of 3-substituted bicyclo[1.1.1]pentyl-1-magnesium and -zinc derivs. The latter have been coupled with various alkenyl, aryl, and biaryl halides and triflates under NiCl<sub>2</sub>dppf, Pd(PPh<sub>3</sub>)<sub>4</sub>, or PdCl<sub>2</sub>(dppf) catalysis to give a number of 1,3-disubstituted bicyclo[1.1.1]pentyl derivs., several of which exhibit liquid crystalline properties, in moderate to very good yields. The coupling products have been further transformed to yield bicyclo[1.1.1]pentyl derivs. bearing alkynyl, cyano, and/or alkenyl groups.

IT 144292-48-8

RL: RCT (Reactant); RACT (Reactant or reagent)

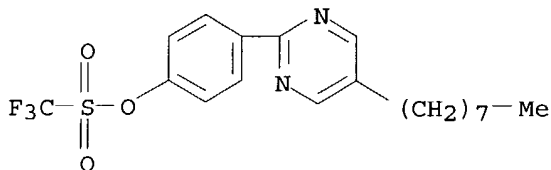
(nickel- and palladium-catalyzed cross-coupling reactions at the bridgehead of bicyclo[1.1.1]pentane derivs.)

RN 144292-48-8 CAPLUS



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CN Methanesulfonic acid, trifluoro-, 4-(5-octyl-2-pyrimidinyl)phenyl ester  
(9CI) (CA INDEX NAME)



REFERENCE COUNT: 82 THERE ARE 82 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 20 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:791837 CAPLUS

DOCUMENT NUMBER: 132:28756

TITLE: Monostable ferroelectric active matrix display

INVENTOR(S): Wingen, Rainer; Nonaka, Toshiaki; Hornung, Barbara

PATENT ASSIGNEE(S): Aventis Research and Technologies GmbH and Co. KG, Germany

SOURCE: Ger. Offen., 18 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19825484	A1	19991209	DE 1998-19825484	19980608
WO 9964538	A1	19991216	WO 1999-EP3939	19990608
W: BR, CA, CN, CZ, HU, JP, KR, MX, PL, RU, US				
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 1086194	A1	20010328	EP 1999-929151	19990608
EP 1086194	B1	20030521		
R: DE, FR, GB				
JP 2002517598	T2	20020618	JP 2000-553530	19990608
US 6551668	B1	20030422	US 2001-719028	20010309
PRIORITY APPLN. INFO.:			DE 1998-19825484 A	19980608
			DE 1998-19830203 A	19980707
			WO 1999-EP3939 W	19990608

OTHER SOURCE(S): MARPAT 132:28756

AB The monostable ferroelec. active matrix display contains liquid crystals represented by R1(A1M1)a(A2M2)bA3(M4A4)c(A5M5)dR2 [A3 = fluorinated aromatic ring(s); R1, R2 = H, C2-12-alkyl, alkoxy, etc.; A1, A2, A4, A5 = 1,4-phenylene, 1,3-phenylene, cyclohex-1-en-1,4-diyl, cyclohex-2-en-1,4-diyl, etc.; M1, M2, M3, M5 = single cond, OCO, COO, OCH2, CH2O, CH2CH2, CH2CH2CH2CH2, C.tplbond.C; a, b, c, d = 0, 1], R3(A7M7)a(A8M8)bA6(M9A9)c(A10M10)dR4 [A6 = ring(s); R3, R4 = H, C2-12-alkyl, alkoxy, etc.; A7, A8, A9, A10 = 1,4-phenylene, 1,3-phenylene, cyclohex-1-en-1,4-diyl, cyclohex-2-en-1,4-diyl, etc.; M7, M8, M9, M10 = single cond, OCO, COO, OCH2, CH2O, CH2CH2, CH2CH2CH2CH2, C.tplbond.C; a, b, c, d = 0, 1], R5(A11M11)a(A12M12)bA13 [A13 = substituted **phenyl**; R5 = H, C2-12-alkyl, alkoxy, etc.; A11, A12 = 1,4-phenylene, 1,3-phenylene, cyclohex-1-en-1,4-diyl, cyclohex-2-en-1,4-diyl, etc.; M11, M12 = single cond, OCO, COO, OCH2, CH2O, CH2CH2, CH2CH2CH2CH2, C.tplbond.C; a, b, c, d = 0, 1], and R6(A14M14)a(A15M15)b(M16A16)c(A17M17)dM18R7 [R6 = H, C2-12-alkyl, alkoxy, etc.; R7 = C3-12-alkyl, etc.; A14-17 = 1,4-phenylene, 1,3-phenylene, cyclohex-1-en-1,4-diyl, cyclohex-2-en-1,4-diyl, etc.; M14-17 = single cond, OCO, COO, OCH2, CH2O,

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CH<sub>2</sub>CH<sub>2</sub>, CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>, C.tplbond.C; M18 = single cond, OCH<sub>2</sub>, CH<sub>2</sub>O, etc.; a, b, c, d = 0, 1].

IT 251934-87-9

RL: DEV (Device component use); USES (Uses)

(in liquid crystal mixture of monostable ferroelec. active matrix display)

RN 251934-87-9 CAPLUS

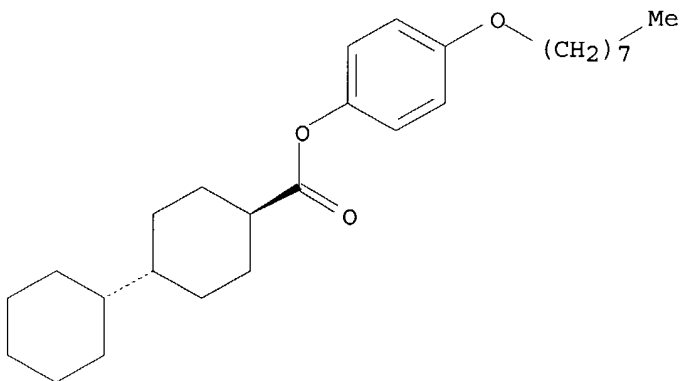
CN [1,1'-Bicyclohexyl]-4-carboxylic acid, 4-(octyloxy)phenyl ester, trans-,  
mixt. with 4-decyl-2,3-difluoro-4''-pentyl-1,1':4',1''-terphenyl,  
2,3-difluoro-4-heptyl-4''-pentyl-1,1':4',1''-terphenyl,  
2',3'-difluoro-4-(hexyloxy)-4''-pentyl-1,1':4',1''-terphenyl,  
2-(4-ethylphenyl)-5-(4-octylphenyl)-1,3,4-thiadiazole,  
2'-fluoro-4-(octyloxy)-4''-pentyl-1,1':4',1''-terphenyl,  
4-[2-(4-hexylphenyl)-5-thiazolyl]phenyl nonanoate and 5-octyl-2-[4-(octyloxy)phenyl]pyrimidine (9CI) (CA INDEX NAME)

CM 1

CRN 251934-86-8

CMF C27 H42 O3

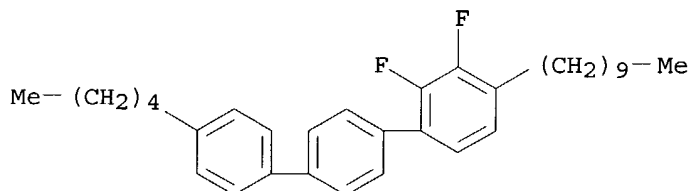
Relative stereochemistry.



CM 2

CRN 251934-85-7

CMF C33 H42 F2

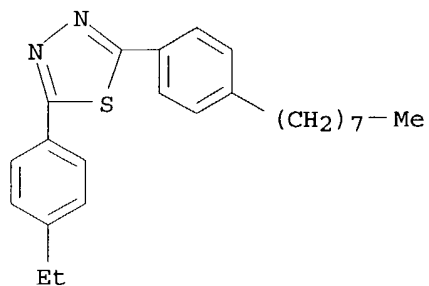


CM 3

CRN 165454-56-8

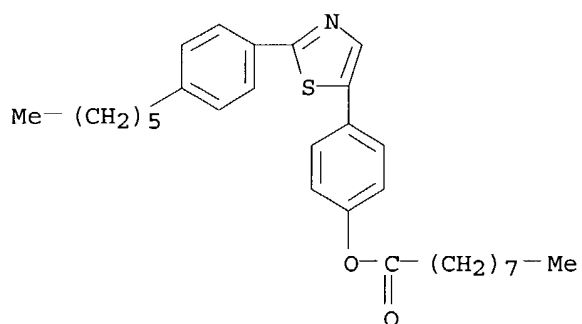
CMF C24 H30 N2 S

09/ 811,359



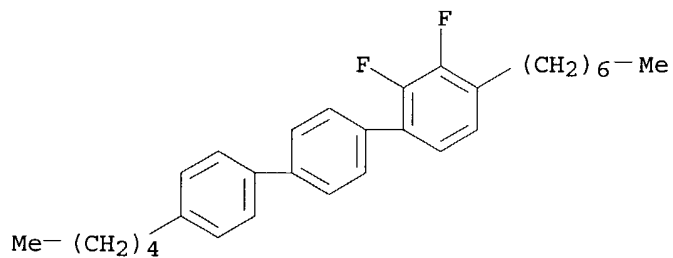
CM 4

CRN 139674-43-4  
CMF C30 H39 N O2 S



CM 5

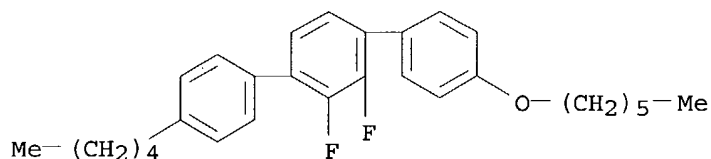
CRN 121218-90-4  
CMF C30 H36 F2



CM 6

CRN 121218-75-5  
CMF C29 H34 F2 O

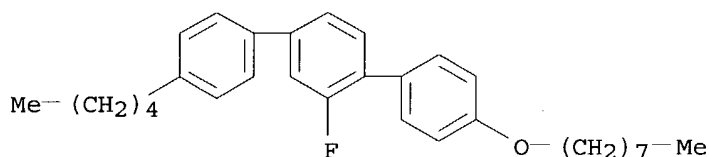
09/ 811,359



CM 7

CRN 117802-11-6

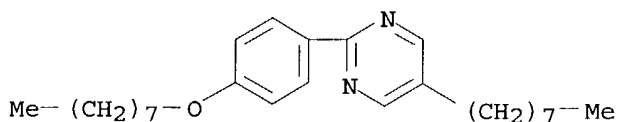
CMF C31 H39 F O



CM 8

CRN 57202-50-3

CMF C26 H40 N2 O



L11 ANSWER 21 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:661479 CAPLUS

DOCUMENT NUMBER: 132:42727

TITLE: Unified surface anchoring energy for cyano- and fluorinated nematic liquid crystals on a polymer alignment layer

AUTHOR(S): Ishihara, Shoichi; Tsuji, Makoto; Sugimura, Akihiko

CORPORATE SOURCE: LCD Development Group, Display Device Development Center, Matsushita Electric Industrial Co., Ltd., Osaka, 570-8501, Japan

SOURCE: Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1999), 329, 773-782

CODEN: MCLCE9; ISSN: 1058-725X

PUBLISHER: Gordon & Breach Science Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The unified surface anchoring energy, which is proposed to describe the generalized anisotropic interaction between the nematic director and the substrate, was studied for nematic slabs of various cyano- and fluorinated liquid crystals (LCs) on a polyimide alignment layer. A saturation voltage method, combined with a conventional optical method, was employed for determining the unified surface anchoring energy. The surface anchoring strength (SAS) was found to vary over the range 10<sup>-4</sup> to 10<sup>-3</sup> [J/m<sup>2</sup>]

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depending on the LC mol. structure. It was also found that the values of SAS change with respect to the tilt angle in opposite directions for the cyano- and fluorinated LCs.

IT 252328-57-7

RL: PRP (Properties)

(surface anchoring strength on polyimide alignment layer)

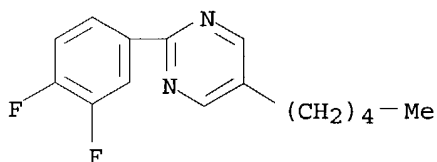
RN 252328-57-7 CAPLUS

CN Pyrimidine, 5-butyl-2-(4'-fluoro[1,1'-biphenyl]-4-yl)-, mixt. with 2-(3,4-difluorophenyl)-5-pentylpyrimidine, 2-(3,4-difluorophenyl)-5-propylpyrimidine and 2-(4'-fluoro[1,1'-biphenyl]-4-yl)-5-pentylpyrimidine (9CI) (CA INDEX NAME)

CM 1

CRN 107392-37-0

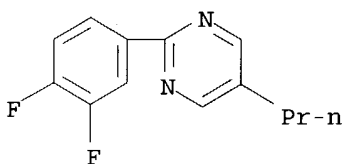
CMF C15 H16 F2 N2



CM 2

CRN 107392-35-8

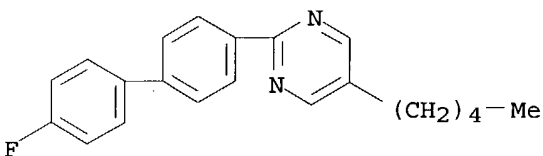
CMF C13 H12 F2 N2



CM 3

CRN 95495-18-4

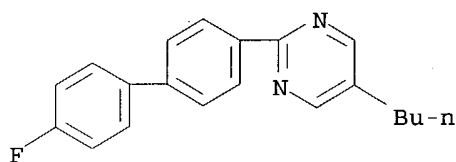
CMF C21 H21 F N2



CM 4

CRN 95495-17-3

CMF C20 H19 F N2



REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 22 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:661467 CAPLUS

DOCUMENT NUMBER: 132:7733

TITLE: Smectic layering at the free surface of isotropic liquid crystals in the pre-smectic temperature region characterized by ellipsometry

AUTHOR(S): Glorieux, Christ; De Schrijver, Peter; Johnson, Patrick M.; Balus, Oana; Serban, Constantin; Huang, Cheng Cher; Thoen, Jan

CORPORATE SOURCE: Laboratorium voor Akoestiek en Thermische Fysica, Departement Natuurkunde, K.U. Leuven, Louvain, B-3001, Belg.

SOURCE: Molecular Crystals and Liquid Crystals Science and Technology, Section A: Molecular Crystals and Liquid Crystals (1999), 329, 663-670

CODEN: MCLCE9; ISSN: 1058-725X

PUBLISHER: Gordon & Breach Science Publishers

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The angular dependence of the ellipsometric signal of bulk isotropic dodecylcyanobiphenyl (12CB) as a function of temperature in the pre-smectic temperature region was determined. Using a simple model, the order parameter of the discontinuously growing smectic surface layer was determined approaching the isotropic-smectic phase transition temperature. Also the pretransitional isotropic region of the isotropic-smectic transition of the liquid crystal compound 2-(4-(1,1-dihydro-2-(2-perfluorobutoxy)perfluoroethoxy)perfluoroethoxy)phenyl-5-octylpyrimidine (H8F(4,2,1)MOPP) was studied.

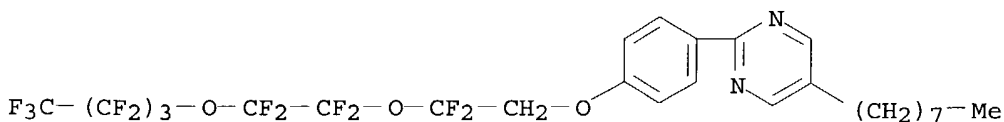
IT 152914-98-2, 2-(4-(1,1-Dihydro-2-(2-perfluorobutoxy)perfluoroethoxy)perfluoroethoxy)phenyl-5-octylpyrimidine

RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(smectic layering at free surface of isotropic liquid crystals in pre-smectic temperature region characterized by ellipsometry)

RN 152914-98-2 CAPLUS

CN Pyrimidine, 2-[4-[2,2-difluoro-2-[1,1,2,2-tetrafluoro-2-(nonafluorobutoxy)ethoxy]ethoxy]phenyl]-5-octyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 23 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:567096 CAPLUS

DOCUMENT NUMBER: 132:102399

TITLE: Synthesis and antitumor activity of N'-(benzylidene-

and ethylidene)hydrazides of 2-hydroxy- and 2-**phenyl**-6-hydroxy-4-methylpyrimidyl-5-acetic acids

AUTHOR(S): Khachatryan, V. E.; Israelyan, S. G.; Stepanyan, G. M.; Arsenyan, F. G.; Garibjanyan, B. T.; Melik-Ohanjanyan, R. G.

CORPORATE SOURCE: Inst. Tonkoi Org. Khim. im. A.A. Mndzhoyana, NAN Respubl. Arm., Yerevan, Armenia

SOURCE: Khimicheskii Zhurnal Armenii (1999), 52(1-2), 102-106  
CODEN: KZARF3

PUBLISHER: Izdatel'stvo Gitutyun NAN Respubliki Armenii

DOCUMENT TYPE: Journal

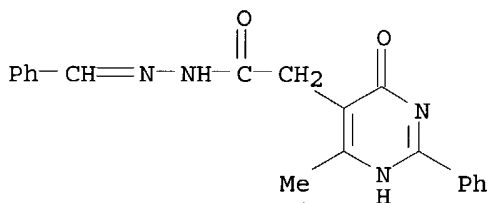
LANGUAGE: Russian

AB The series of N'-(benzylidene- and ethylidene)hydrazides of 2-hydroxy- and 2-**phenyl**-6-hydroxy-4-methylpyrimidyl-5-acetic acids were synthesized by the i reaction of appropriate hydrazides with aromatic aldehydes or ketones in ethanol or DMF in the presence of catalytic amts. of concentrated hydrochloric acid. The structure of newly obtained compds. was proved by UR-, NMR- and mass spectroscopy. Toxicity and antitumor activity of these compds. was investigated. The majority of them showed low toxicity and moderate antitumor activity on Sa-45, Sa-37, WCS exptl. tumors. The p-fluorobenzylidene hydrazide of met-acyl-5-acetic acid and p-bromoethylidene hydrazide of 2-**phenyl**-4-hydroxy-6-methylpyrimidyl-5-acetic acid were the most active compds. These substances showed moderate activity on LLC and was non-effective against La hemocytoblastosis.

IT 255867-67-5P  
RL: ADV (Adverse effect, including toxicity); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(synthesis and antitumor activity of benzylidene- and ethylidene-hydrazides of hydroxy- and phenylhydroxymethylpyrimidylacetic acids)

RN 255867-67-5 CAPLUS

CN 5-Pyrimidineacetic acid, 1,4-dihydro-6-methyl-4-oxo-2-phenyl-, (phenylmethylene)hydrazide (9CI) (CA INDEX NAME)



L11 ANSWER 24 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:358691 CAPLUS

DOCUMENT NUMBER: 131:109179

TITLE: Smectic A and C materials with novel director tilt and layer thickness behavior

AUTHOR(S): Radcliffe, Marc D.; Brostrom, Myles L.; Epstein, Kenneth A.; Rappaport, Aaron G.; Thomas, Britt N.; Shao, Renfan; Clark, Noel A.

CORPORATE SOURCE: 3M Company, St. Paul, MN, 55144, USA

SOURCE: Liquid Crystals (1999), 26(6), 789-794  
CODEN: LICRE6; ISSN: 0267-8292

PUBLISHER: Taylor & Francis Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The authors report a smectic liquid crystal in which a tilt of the mol.

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orientation away from the layer normal in the Smectic C phase of up to 240 occurs with minimal layer contraction. This characteristic, accompanied by an exceptionally large underlying neg. thermal layer expansion coefficient, enables the formation of chiral smectic electrooptical cells having nearly the ideal 'bookshelf' layer geometry, free from the complexities of the chevron layer structure produced by contraction.

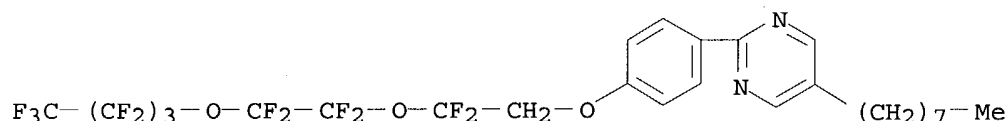
IT 152914-98-2, 2-{4-[1,1-Dihydro-2-(2-perfluorobutoxyperfluoroethoxy)perfluoroethoxy]}phenyl-5-octylpyrimidine

RL: PRP (Properties)

(director tilt away from layer normal in relation to layer thickness behavior in smectic C and A liquid crystals in relation to formation of chiral smectic electrooptical cells with bookshelf layer geometry)

RN 152914-98-2 CAPLUS

CN Pyrimidine, 2-[4-[2,2-difluoro-2-[1,1,2,2-tetrafluoro-2-(nonafluorobutoxy)ethoxy]ethoxy]phenyl]-5-octyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 21 THERE ARE 21 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 25 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:225668 CAPLUS

DOCUMENT NUMBER: 130:252374

TITLE: Preparation of optically active 3-fluoroalkylphenylpyrimidines for ferroelectric liquid crystals

INVENTOR(S): Kusumoto, Tetsuo; Kato, Miho; Sato, Kenichi; Hiyama, Tamejiro

PATENT ASSIGNEE(S): Sagami Chemical Research Center, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

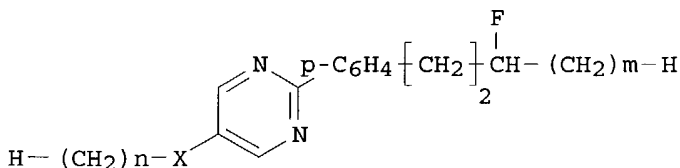
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11092457	A2	19990406	JP 1997-259515	19970925
PRIORITY APPLN. INFO.:			JP 1997-259515	19970925
OTHER SOURCE(S):		CASREACT 130:252374; MARPAT 130:252374		

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I

AB Title compds. I ( $m = 1-16$ ;  $n = 1-20$ ;  $X = \text{single bond, O}$ ), useful as ferroelec. liquid crystal materials (no data), are prepared by reaction of 4-methylbenzonitrile with optically active  $\text{Q}(\text{CH}_2)_m\text{H}$  ( $\text{Q} = \text{oxiranyl}$ ;  $m =$



1-16) in the presence of bases, fluorination of optically active p-NCC6H4CH2CH2CH(OH)(CH2)mH (m = 1-16), reaction of optically active p-NCC6H4CH2CH2CHF(CH2)mH (m = 1-16) with hydrogen halides and alcs., reaction with NH3, reaction with H(CH2)nXC(CHO):CHNMe2 (n, X = same as I). 4-Methylbenzonitrile was reacted with (R)-1,2-epoxyoctane in the presence of (i-Pr)2NH and BuLi in THF at room temperature for 2 h and fluorinated with Et2NSF3 in CH2Cl2 at room temperature to give (S)-4-(3-fluorononyl)benzonitrile, which was reacted with HCl and EtOH in CH2Cl2-ether at room temperature for 4 h, reacted with NH3 at room temperature for 5 days, and cyclized with 3-(N,N-dimethylamino)-2-octyloxyacrolein in a NaOMe/MeOH solution under reflux overnight to give 36% (S)-2-[4-(3-fluorononyl)phenyl]-5-octyloxy-pyrimidine.

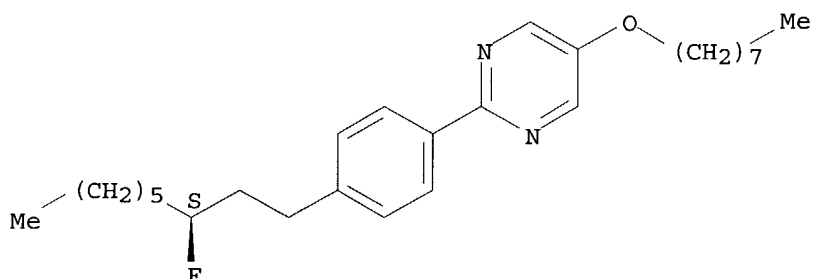
IT 152291-78-6P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses) (preparation of optically active fluoroalkylphenylpyrimidines by ring opening of oxiranes with methylbenzonitrile, fluorination, and cyclization)

RN 152291-78-6 CAPLUS

CN Pyrimidine, 2-[4-[(3S)-3-fluorononyl]phenyl]-5-(octyloxy)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 26 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1999:121831 CAPLUS

DOCUMENT NUMBER: 130:318814

TITLE: Designing banana-shaped liquid crystals without Schiff's base units: m-terphenyls, 2,6-diphenylpyridines and V-shaped tolane derivatives

AUTHOR(S): Shen, Dong; Diele, Siegmund; Pelzl, Gerhard; Wirth, Ina; Tschierske, Carsten

CORPORATE SOURCE: Institut für Organische Chemie, Martin-Luther-Universität Halle-Wittenberg, Halle, D-06120, Germany

SOURCE: Journal of Materials Chemistry (1999), 9(3), 661-672  
CODEN: JMACEP; ISSN: 0959-9428

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

AB This paper reports attempts to obtain (anti)ferroelec. switchable achiral banana-shaped mols. without Schiff's base units. For this purpose the authors synthesized novel V-shaped mols. consisting of rigid angular central units [1,3-disubstituted benzene, 2,7-disubstituted naphthalene, 1,3-diphenylbenzene, 2,6-diphenylnitrobenzene, 2,6-diphenylpyridine, 1,3-bis(phenylethynyl)benzene, 1-phenyl-3-(phenylethynyl)benzene] connected via ester linkages to two rigid cores (1,4-disubstituted benzenes, biphenyls, 2-phenylpyrimidines, phenylbenzoates). Most compds. have rather high m.ps. Only mols. with seven aromatic rings show liquid crystalline properties. Two-dimensional modulated smectic phases (rectangular columnar phases) were found for mols. with

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phenylbenzoate rigid units. Intercalated fluid smectic phases were detected for the corresponding 2-phenylpyrimidine derivs. For the 1st time in the case of banana-shaped mols. a nematic phase was observed for a 2'-nitro-m-terphenyl-4,4''-diyl bisbenzoate. However, none of the synthesized compds. exhibit the typical texture of the (anti)ferroelec. switchable mesophases, known from the Schiff's base derivs.

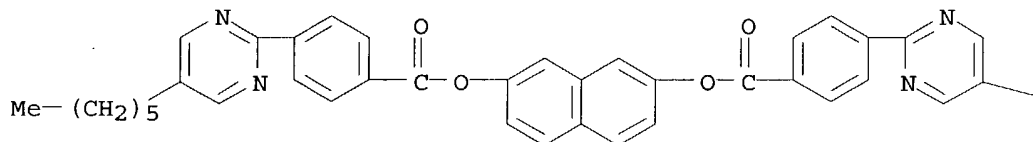
IT 223654-83-9P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
(preparation and characterization of)

RN 223654-83-9 CAPLUS

CN Benzoic acid, 4-(5-hexyl-2-pyrimidinyl)-, 2,7-naphthalenediyl ester (9CI)  
(CA INDEX NAME)

PAGE 1-A



PAGE 1-B

(CH<sub>2</sub>)<sub>5</sub>-Me

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 27 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:535947 CAPLUS

DOCUMENT NUMBER: 129:223608

TITLE: Smectic liquid-crystal composition for information recording media

INVENTOR(S): Fukumasa, Mitsumutsu; Okada, Tomomi; Yoshisawa, Atsushi

PATENT ASSIGNEE(S): Japan Energy K. K., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

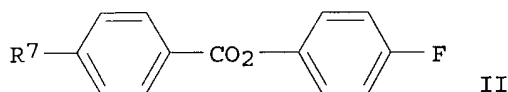
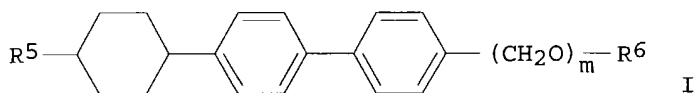
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10219251	A2	19980818	JP 1997-42890	19970213
PRIORITY APPLN. INFO.:			JP 1997-42890	19970213
OTHER SOURCE(S):		MARPAT 129:223608		

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AB The media have (A) 4-alkyl-4-cyanobiphenyl and/or 4-alkoxy-4-cyanobiphenyl and (B) R1A1CO2CH2CH(Me) (CH2)nCH(Me)CH2OCOB1R2, R3A2OCOCH(Me)CH2CO2B2R4, I, and/or II (R1-7 = alkyl, alkoxy; A1, B1, A2, B2 = phenylpyrimidine, biphenyl, **phenyl**:benzoic acid, phenylcyclohexane, **phenyl**:biphenylcarboxylic acid, biphenyl:benzoic acid, terphenylpyrimidine, 1,5-diphenylpyrimidine; n = 3-15 integer; m = 0, 1). The composition displays phase transformation by lower voltage application. The composition is useful for high quality and high contrast information recording such as an electrophotog. material, an optical sensor, etc.

IT **212554-10-4**

RL: DEV (Device component use); USES (Uses)

(liquid crystal mixture; nematic liquid crystal mixture containing alkyl or alkoxy cyanobiphenyl for information recording media)

RN 212554-10-4 CAPLUS

CN Benzoic acid, 4-(5-octyl-2-pyrimidinyl)-, (2S,9S)-2,9-dimethyl-1,10-decanediyl ester, mixt. with 4'-dodecyl[1,1'-biphenyl]-4-carbonitrile, 4'-nonyl[1,1'-biphenyl]-4-carbonitrile and 4'-(nonyloxy)[1,1'-biphenyl]-4-carbonitrile (9CI) (CA INDEX NAME)

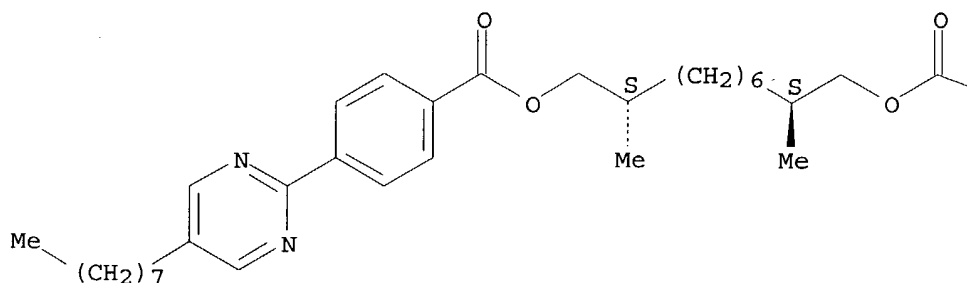
CM 1

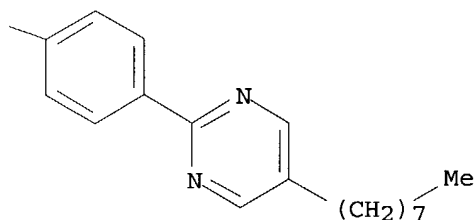
CRN 212554-09-1

CMF C50 H70 N4 O4

Absolute stereochemistry.

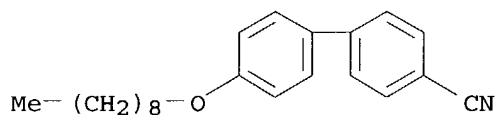
PAGE 1-A





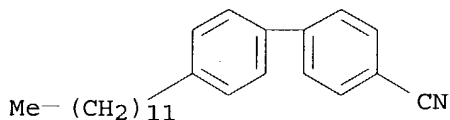
CM 2

CRN 58932-13-1  
CMF C22 H27 N O



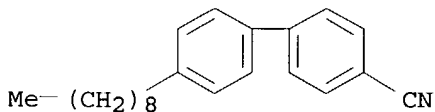
CM 3

CRN 57125-49-2  
CMF C25 H33 N



CM 4

CRN 52709-85-0  
CMF C22 H27 N



L11 ANSWER 28 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:385479 CAPLUS

DOCUMENT NUMBER: 129:54375

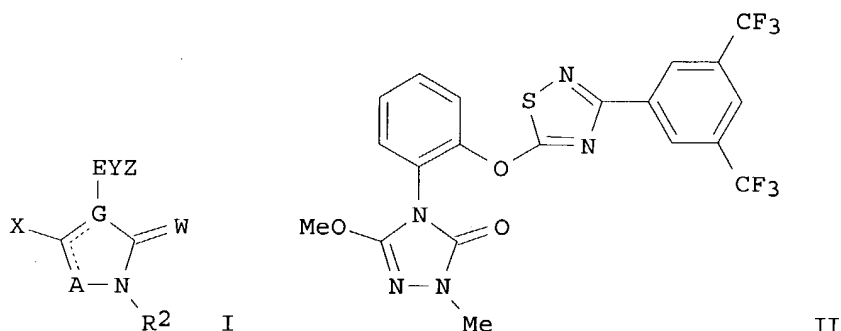
TITLE: Arthropodocidal and fungicidal cyclic amides  
[triazolones] and their preparation, use, and  
compositions

INVENTOR(S): Brown, Richard James; Chan, Dominic Ming-Tak; Howard,  
Michael Henry, Jr.; Daniel, Dilon Jancey; Clark, David

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PATENT ASSIGNEE(S): Alan; Selby, Thomas Paul  
SOURCE: E. I. Du Pont de Nemours & Co., USA  
PCT Int. Appl., 232 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9823155	A1	19980604	WO 1996-US18916	19961126
W: JP, KR				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
ZA 9709943	A	19990505	ZA 1997-9943	19971105
WO 9823156	A1	19980604	WO 1997-US21944	19971125
W: AL, AM, AU, AZ, BA, BB, BG, BR, BY, CA, CN, CU, CZ, EE, GE, HU, ID, IL, IS, JP, KG, KP, KR, KZ, LC, LK, LR, LT, LV, MD, MG, MK, MN, MX, NO, NZ, PL, RO, RU, SG, SI, SK, SL, TJ, TM, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9854633	A1	19980622	AU 1998-54633	19971125
EP 944314	A1	19990929	EP 1997-948597	19971125
R: CH, DE, DK, ES, FR, GB, IT, LI, NL, IE				
BR 9713415	A	20000418	BR 1997-13415	19971125
JP 2001506984	T2	20010529	JP 1998-524889	19971125
MX 9904789	A	20000131	MX 1999-4789	19990524
PRIORITY APPLN. INFO.:			WO 1996-US18916	A 19961126
			US 1996-33614P	P 19961219
			US 1997-48844P	P 19970606
			WO 1997-US21944	W 19971125
OTHER SOURCE(S):		MARPAT 129:54375		
GI				



AB Title compds. I and their N-oxides and agriculturally suitable salts are disclosed [wherein E = (un)substituted 1,2-phenylene, naphthalene or heterocyclyl; A = O, S, N, NR<sub>3</sub> or CR<sub>4</sub>; G = C or N; when G is C, then A is O, S or NR<sub>3</sub> and the floating double bond is attached to G; and when G is N, than A is N or CR<sub>4</sub> and the floating double bond is attached to A; W = O, S, NH, N(C1-C6 alkyl) or NO(C1-C6 alkyl); X = H, OR<sub>1</sub>, SOMR<sub>1</sub>, halo, C1-C6 alkyl, C1-C6 haloalkyl, C3-C6 cycloalkyl, cyano, NH<sub>2</sub>, NHR<sub>1</sub>, N(C1-C6 alkyl)R<sub>1</sub>, NH(C1-C6 alkoxy) or N(C1-C6 alkoxy)R<sub>1</sub>; R<sub>2</sub> = H, C1-C6 alkyl, C1-C6 haloalkyl, C2-C6 haloalkyl, C2-C6 alkenyl, C2-C6 haloalkenyl, C2-C6

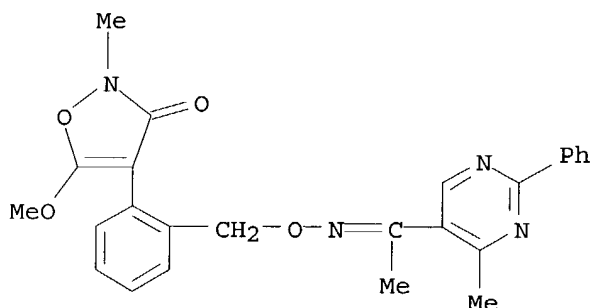
alkynyl, C2-C6 haloalkynyl, C3-C6 cycloalkyl, C2-C4 alkylcarbonyl, C2-C6 alkoxy carbonyl, hydroxy, C1-C2 alkoxy, or acetyloxy; R1= (halo)alkyl, (halo)alkenyl, etc.; R3= H, (halo)alkyl, etc.; Y = O, CO, SO, etc.; Z = (un)substituted alkyl, alkenyl or alkynyl, R4 = H, halo, alkyl, etc.; m = 0, 1 or 2]. Claims cover methods of arthropod and fungal control, novel compds., arthropodicidal and fungicidal compns., and novel intermediates. Approx. 1000 invention compds. were prepared For instance, 5-chloro-2,4-dihydro-4-(2-methoxyphenyl)-2-methyl-3H-1,2,4-triazol-3-one (preparation given) underwent a sequence of cleavage of the Me ether with BBr<sub>3</sub>, methoxylation of the chloride with NaOMe, and etherification of the phenolic hydroxy group with 5-chloro-3-[3,5-bis(trifluoromethyl)phenyl]-1,2,4-thiadiazole, to give title compound II. Selected I were active in screens against Erysiphe graminis, Pyricularia oryzae, Spodoptera frugiperda, Tetranychus urticae, and a variety of other standard pests.

IT 185336-64-5P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation as arthropodicide and fungicide)

RN 185336-64-5 CAPLUS

CN 3(2H)-Isoxazolone, 5-methoxy-2-methyl-4-[2-[[[1-(4-methyl-2-phenyl-5-pyrimidinyl)ethylidene]amino]oxy]methyl]phenyl]- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 29 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:351919 CAPLUS

DOCUMENT NUMBER: 129:87956

TITLE: Color diffusion transfer image-forming system and color image formation

INVENTOR(S): Naruse, Hideaki; Nakamura, Takemare

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 82 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10142764	A2	19980529	JP 1996-317058	19961113
PRIORITY APPLN. INFO.:			JP 1996-317058	19961113

OTHER SOURCE(S): MARPAT 129:87956

GI For diagram(s), see printed CA Issue.

AB In the title system using a photosensitive material containing a photosensitive Ag halide, a binder, a compound I (Z = carbamoyl, acyl,

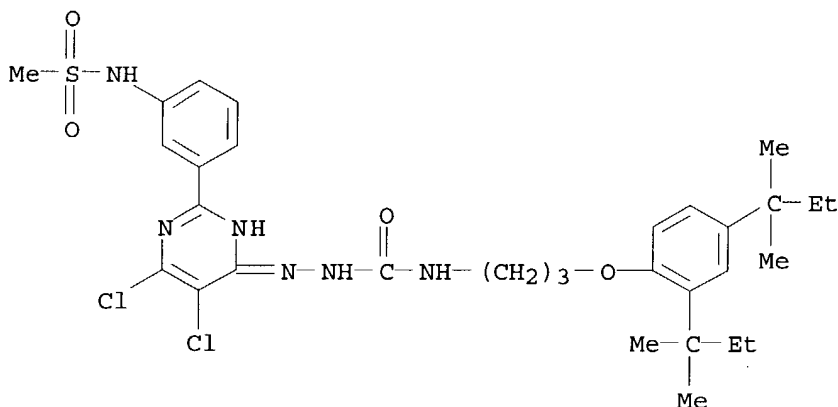
alkoxycarbonyl, aryloxy carbonyl, sulfonyl, sulfamoyl; Q = atoms required to form an unsatd. ring along with the C atom), and a compound that reacts with an oxidized product of I to form or release a diffusive dye on a support and a dye-fixing material possessing  $\geq 1$  dye-fixing layer on which the dye formed by exposure and development of the photosensitive material is transferred, the dye-fixing layer and/or its adjacent layer contains  $\geq 1$  selected from phenol derivs., II and III [R10 = alkyl, alkenyl, aryl, aralkyl, heterocycle, R18CO, R19SO<sub>2</sub>, R20NHCO (R18-20 = substituent); R11, R12 = H, halo, alkyl, alkenyl, alkoxy, alkenoxy; R13-17 = H, alkyl, alkenyl, aryl; E = nonmetal atoms required to form a 5- to 7-membered ring along with the C and N atoms; R18 = H, alkyl, alkenyl, alkynyl, acyl, sulfonyl, sulfinyl, oxy radical, OH; R19-22 = H, alkyl]. The photosensitive material is imagewise exposed and laminated with the dye-fixing material followed by development to fix the diffusive dye from the photosensitive material on the dye-fixing material to form an image. Durable, high d. color images are obtained.

IT 209247-50-7

RL: TEM (Technical or engineered material use); USES (Uses)  
(diffusion-transfer photog. material containing hydrazine derivative color developer)

RN 209247-50-7 CAPLUS

CN Hydrazinecarboxamide, N-[3-[2,4-bis(1,1-dimethylpropyl)phenoxy]propyl]-2-[5,6-dichloro-2-[3-[(methylsulfonyl)amino]phenyl]-4-pyrimidinyl]- (9CI)  
(CA INDEX NAME)



L11 ANSWER 30 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:341533 CAPLUS

DOCUMENT NUMBER: 129:21744

TITLE: **Phenyl** polyhaloalkyl ether derivatives,  
liquid-crystal composition containing the same, and  
liquid-crystal display element

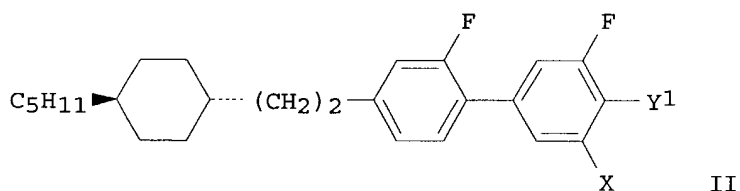
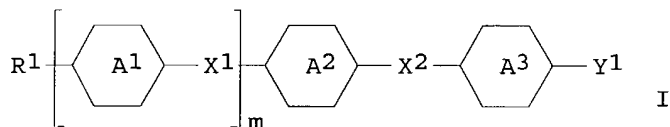
INVENTOR(S): Shibata, Kouichi; Matsui, Shuichi; Miyazawa,  
Kazutoshi; Takeuchi, Hiroyuki; Hisatsune, Yasusuke;  
Takeshita, Fusayuki; Nakagawa, Etsuo  
PATENT ASSIGNEE(S): Chisso Corp., Japan; Shibata, Kouichi; Matsui,  
Shuichi; Miyazawa, Kazutoshi; Takeuchi, Hiroyuki;  
Hisatsune, Yasusuke; Takeshita, Fusayuki; Nakagawa,  
Etsuo

SOURCE: PCT Int. Appl., 79 pp.  
CODEN: PIXXD2

DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9821172	A1	19980522	WO 1997-JP4114	19971112
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, ID, IL, IS, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
JP 10139709	A2	19980526	JP 1996-316958	19961113
AU 9749642	A1	19980603	AU 1997-49642	19971112
EP 945422	A1	19990929	EP 1997-912427	19971112
R: DE, FR, GB				
US 2001019121	A1	20010906	US 1999-308039	19990713
PRIORITY APPLN. INFO.:			JP 1996-316958	A 19961113
			WO 1997-JP4114	W 19971112

GI



AB Claimed are novel liquid-crystal compds. which have an especially large value of dielec. anisotropy ( $\Delta\epsilon$ ) and a satisfactory compatibility with other liquid-crystal compds. and show a nematic phase in a wide temperature range without detriment to the properties inherent in liquid-crystal fluorine compds.; a liquid-crystal composition containing the same; and a liquid-crystal display element prepared by using the composition. The compds. include Ph polyhaloalkyl ether derivs. represented by general formula [I; wherein X1 and X2 each independently represents 1,2-ethylene, 1,4-butylene, or a covalent bond, provided that not both represent covalent bonds; R1 represents C1-20 alkyl in which at least one methylene group may have been replaced with oxygen, vinylene, or ethynylene; Y1 represents  $\text{OCF}_2\text{CFH}(\text{CF}_2)_n\text{F}$  (wherein n is 0, 1, 2, or 3) or  $\text{OCF}_2\text{Cl}$ ; the rings A1 and A2 each independently represents 1,4-cyclohexylene, 1,4-cyclohexenylene, or 1,4-phenylene and A3 represents 1,4-phenylene, provided that at least one carbon atom in each ring may have been replaced with oxygen or nitrogen and at least one hydrogen atom present on each ring may have been replaced with fluorine or chlorine; m is 0 or 1; and each constituent element of the mol. may contain at least one of the isotopes thereof]. The liquid crystal display element is used for a watch, calculator, various instruments, automobile panel, word processor, electronic note, printer, computer, and TV. Thus, 2-fluoro-4-[2-(trans-4-pentylcyclohexyl)ethyl]boric acid (preparation given) was coupled with 3,5-difluoro-4-(1,1,2,3,3,3-hexafluoropropoxy)bromobenzene in the presence



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of (Ph<sub>3</sub>P)<sub>4</sub>Pd and Na<sub>2</sub>CO<sub>3</sub> in a mixture of toluene and water under reflux for 10 h to give the title compound (II; X = F, Y<sub>1</sub> = OCF<sub>2</sub>CFHCF<sub>3</sub>), which showed phase transition temperature of C 41° N 99.5° I. A liquid crystal composition containing 85 weight% ZLI 1132 and 15 weight% II (X = H, Y<sub>1</sub> = OCF<sub>2</sub>CF<sub>2</sub>H) showed TN<sub>1</sub> at 73.5° and Δε of 10.6 vs. 83.7° and 8.3, resp., for II (X = H, Y<sub>1</sub> = OCF<sub>2</sub>CF<sub>2</sub>H).

IT 175859-31-1

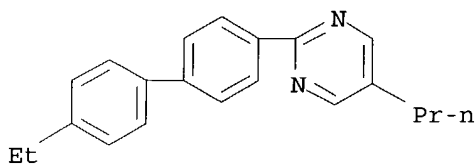
RL: DEV (Device component use); PRP (Properties); TEM (Technical or engineered material use); USES (Uses)

(liquid crystal composition containing; preparation of Ph polyhaloalkyl ether derivs.,

liquid-crystal composition containing them, and liquid-crystal display element)

RN 175859-31-1 CAPLUS

CN Pyrimidine, 2-(4'-ethyl[1,1'-biphenyl]-4-yl)-5-propyl- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 31 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:323239 CAPLUS

DOCUMENT NUMBER: 128:315486

TITLE: Preparation of 2-(4-alkylphenyl)-5-alkylthiadiazoles as liquid crystals

INVENTOR(S): Saito, Shinichi; Shundo, Ryushi; Okabe, Eiji; Saito, Hideo

PATENT ASSIGNEE(S): Chisso Corp., Japan; Saito, Shinichi; Shundo, Ryushi; Okabe, Eiji; Saito, Hideo

SOURCE: PCT Int. Appl., 18 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

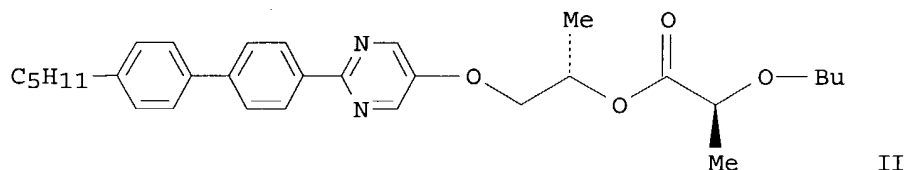
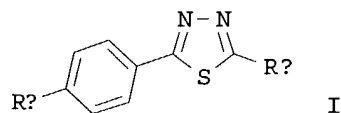
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9820004	A1	19980514	WO 1997-JP3896	19971027
W:	AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, ID, IL, IS, JP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, SL, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
RW:	GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG			
AU 9747245	A1	19980529	AU 1997-47245	19971027
PRIORITY APPLN. INFO.:			JP 1996-307279	19961101
			WO 1997-JP3896	19971027

OTHER SOURCE(S): MARPAT 128:315486

GI



AB The title 2-(4-alkylphenyl)-5-alkylthiadiazoles represented by general formula (I; Ra is C5-C15 alkyl; and Rb is C5-C15 alkyl) are prepared. Claimed are ferroelec. liquid crystal compns. containing I. These compds. are liquid-crystal compds. which are usable as the basic substance of ferroelec. liquid crystal compns., have a low viscosity, and exhibit a liquid crystal phase in a low-temperature region. Thus, Et 4-octylbenzoate was sequentially condensed with hydrazine hydrate and octanoyl chloride to give N-(4-octylbenzoyl)-N'-octanoylhydrazine which was cyclocondensed with Lawesson's reagent to give I (Ra = octyl, Rb = heptyl) (II). II showed phase transition point (Cr 38° Sc 44.6° SA 51.3° Iso). A ferroelec. liquid crystal composition containing II (50 weight%) and a mixture of

6 phenylpyrimidine derivs. (45 weight%) and a chiral dopant (III) (5 weight%) showed phase transition point (room temperature-Sc\* 54.4 SA 58.9 Iso) and response speed 30.0  $\mu$ s at 44.4° in a liquid crystal cell (2  $\mu$ m thickness).

IT 206551-21-5

RL: TEM (Technical or engineered material use); USES (Uses)  
(preparation of (alkylphenyl)alkylthiadiazoles as liquid crystals for ferroelec. liquid crystal compns.)

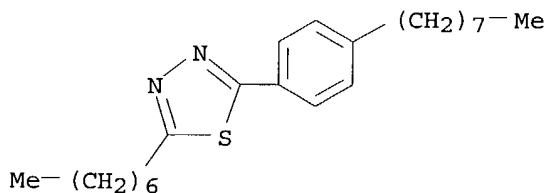
RN 206551-21-5 CAPLUS

CN Propanoic acid, 2-butoxy-, (1S)-1-methyl-2-[[2-(4'-pentyl[1,1'-biphenyl]-4-yl)-5-pyrimidinyl]oxy]ethyl ester, (2S)-, mixt. with 2-[4-(decyloxy)phenyl]-5-octylpyrimidine, 2-(4'-heptyl[1,1'-biphenyl]-4-yl)-5-hexylpyrimidine, 5-heptyl-2-[4-(nonyloxy)phenyl]pyrimidine, 2-heptyl-5-(4-octylphenyl)-1,3,4-thiadiazole, 2-[4-(hexyloxy)phenyl]-5-octylpyrimidine, 5-hexyl-2-(4'-pentyl[1,1'-biphenyl]-4-yl)pyrimidine and 5-octyl-2-[4-(octyloxy)phenyl]pyrimidine (9CI) (CA INDEX NAME)

CM 1

CRN 206550-94-9

CMF C23 H36 N2 S

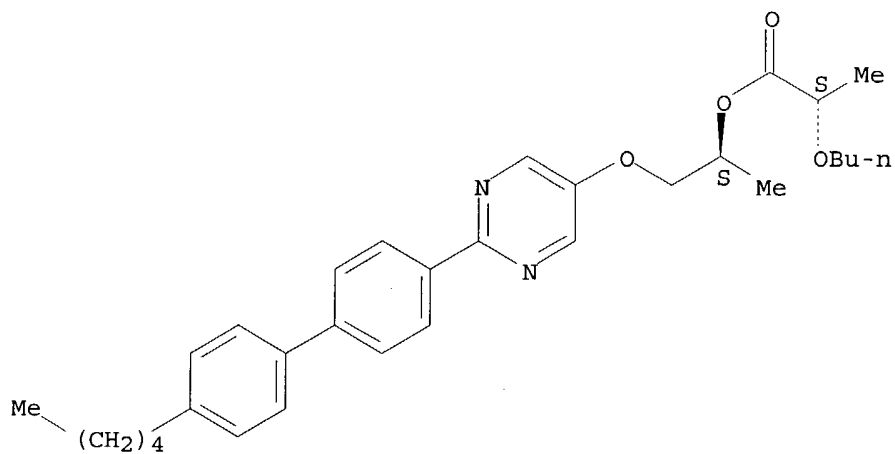


CM 2

09/ 811,359

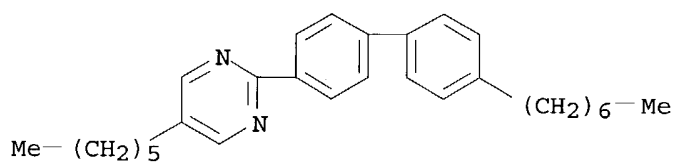
CRN 119218-09-6  
CMF C31 H40 N2 O4

Absolute stereochemistry.



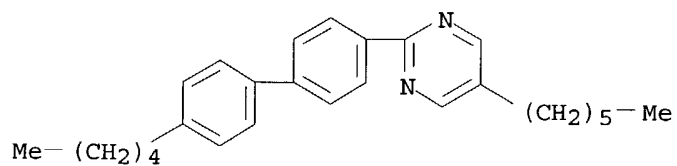
CM 3

CRN 92519-52-3  
CMF C29 H38 N2



CM 4

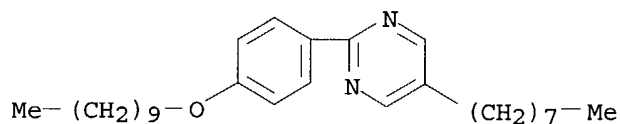
CRN 92178-46-6  
CMF C27 H34 N2



CM 5

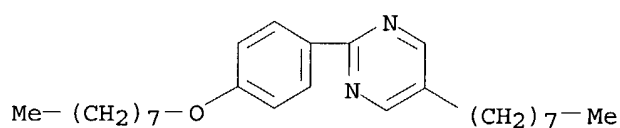
CRN 57202-52-5  
CMF C28 H44 N2 O

09/ 811,359



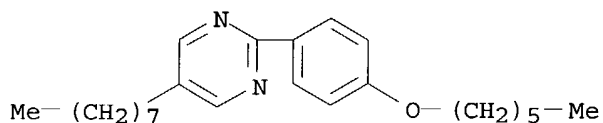
CM 6

CRN 57202-50-3  
CMF C26 H40 N2 O



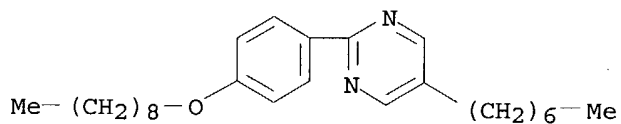
CM 7

CRN 57202-48-9  
CMF C24 H36 N2 O



CM 8

CRN 57202-40-1  
CMF C26 H40 N2 O



REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 32 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:108200 CAPLUS

DOCUMENT NUMBER: 128:210966

TITLE: Manufacture of ferroelectric liquid-crystal composition for display

INVENTOR(S): Takiguchi, Takao; Nakamura, Shinichi; Utakewa, Masako

PATENT ASSIGNEE(S): Canon K. K., Japan

SOURCE: Jpn. Kokai Tokyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

09/ 811,359

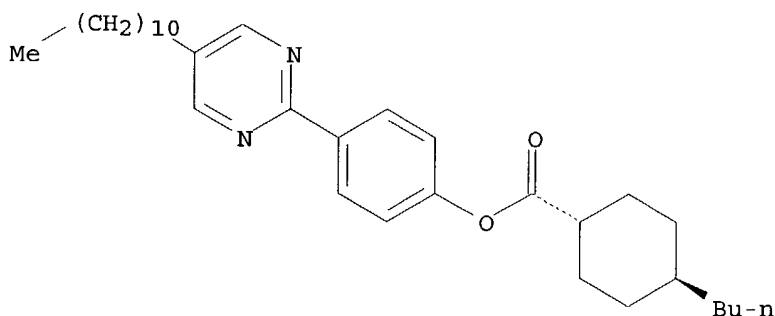
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
	JP 10046149	A2	19980217	JP 1996-216983	19960731
PRIORITY APPLN. INFO.:				JP 1996-216983	19960731
AB	The manufacturing method involves the processes of (1) purifying $\geq 1$ liquid-crystal compound by using 10-50 weight% (vs. the compound) active C and (2) mixing the purified compound with other components for the liquid-crystal composition. The composition shows good switching property in a uniform state and gives high-contrast images.				
IT	204079-42-5				
	RL: DEV (Device component use); USES (Uses) (purification of liquid-crystal compound by active carbon in manufacture of ferroelec. liquid-crystal composition for display)				
RN	204079-42-5 CAPLUS				
CN	Cyclohexanecarboxylic acid, 4-butyl-, 4-(5-undecyl-2-pyrimidinyl)phenyl ester, trans-, mixt. with 5-decyl-2-[4-[(2-fluorooctyl)oxy]phenyl]pyrimidine, 5-dodecyl-2-[4-[(2-fluorooctyl)oxy]phenyl]pyrimidine, 2-[4-(hexyloxy)phenyl]-5-nonylpyrimidine, 2-[4-(hexyloxy)phenyl]-5-octylpyrimidine, 2-[4-(nonyloxy)phenyl]-5-octylpyrimidine, trans-4-(5-undecyl-2-pyrimidinyl)phenyl 4-pentylcyclohexanecarboxylate and trans-4-(5-undecyl-2-pyrimidinyl)phenyl 4-propylcyclohexanecarboxylate (9CI) (CA INDEX NAME)				
CM	1				
CRN	121639-89-2				
CMF	C32 H48 N2 O2				

Relative stereochemistry.



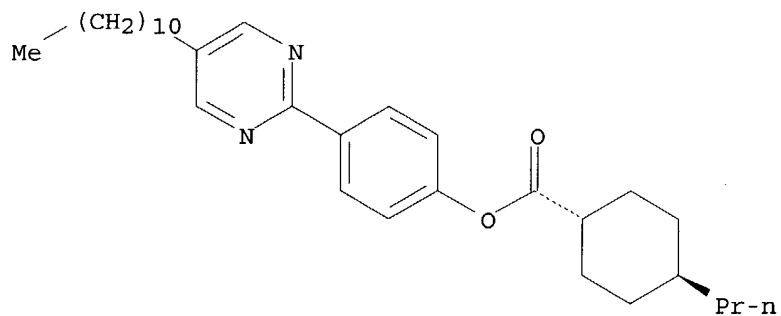
CM 2

CRN 121639-88-1

CMF C31 H46 N2 O2

Relative stereochemistry.

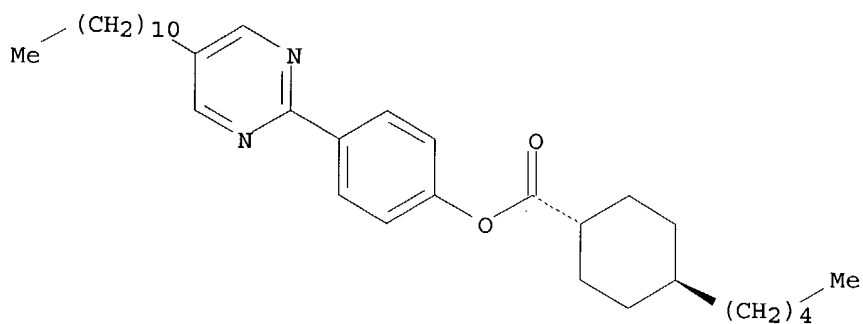
09/ 811,359



CM 3

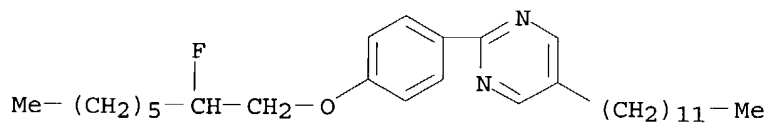
CRN 121083-94-1  
CMF C33 H50 N2 O2

Relative stereochemistry.



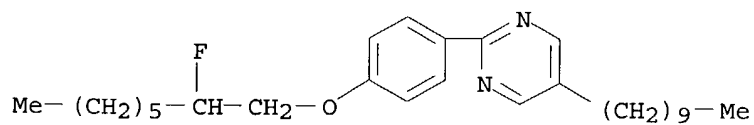
CM 4

CRN 116529-05-6  
CMF C30 H47 F N2 O



CM 5

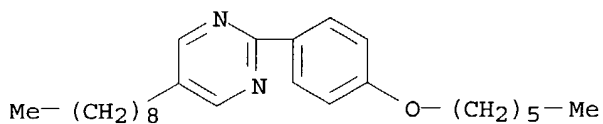
CRN 113701-90-9  
CMF C28 H43 F N2 O



CM 6

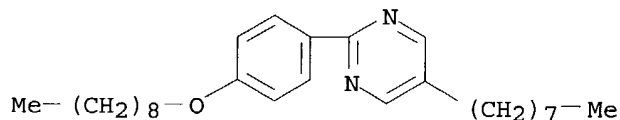
09/ 811,359

CRN 57202-56-9  
CMF C25 H38 N2 O



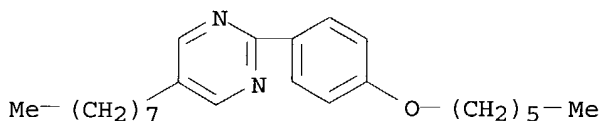
CM 7

CRN 57202-51-4  
CMF C27 H42 N2 O



CM 8

CRN 57202-48-9  
CMF C24 H36 N2 O



L11 ANSWER 33 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1998:90219 CAPLUS  
DOCUMENT NUMBER: 128:225733  
TITLE: Anti-Pneumocystis carinii pneumonia activity of  
dicationic diaryl methylpyrimidines  
AUTHOR(S): Boykin, D. W.; Kumar, A.; Bajic, M.; Xiao, G.; Wilson,  
W. D.; Bender, B. C.; McCurdy, D. R.; Hall, J. E.;  
Tidwell, R. R.  
CORPORATE SOURCE: Department of Chemistry and Center for Biotechnology  
and Drug Design, Georgia State University, Atlanta,  
GA, 30303-3083, USA  
SOURCE: European Journal of Medicinal Chemistry (1997),  
32(12), 965-972  
CODEN: EJMCA5; ISSN: 0223-5234  
PUBLISHER: Editions Scientifiques et Medicales Elsevier  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Synthesis of 2,4-bis(4-amidinophenyl)-5-methylpyrimidine 5,  
2,4-bis[(4-imidazolin-2-yl)phenyl]-6-methylpyrimidine 5,  
2,4-bis[(4-N-i-propylamidino)phenyl]-6-methylpyrimidine 7, and  
2,4-bis[(4-N-isopentylamidino)phenyl]-6-methylpyrimidine 8  
starting from 4-bromobenzamidine and 4'-bromoacetophenone is reported.

The synthesis of 2,4-bis-(4-amidinophenyl)-5-methylpyrimidine 12 and 2,4-bis-[(4-imidazolin-2-yl)**phenyl**]-5-methylpyrimidine 13, also beginning with 4-bromobenzamidine and 4'-bromo-propiophenone is described. A synthesis of 4,6-bis-(4-amidinophenyl)-2-methylpyrimidine 17, 4,6-bis-[(4-imidazolin-2-yl)**phenyl**]-2-methylpyrimidine 18, 4,6-bis[4-Ni-isopropylamidino)**phenyl**]-2-methylpyrimidine 19 and 4,6-bis[(4-N-n-propylamidino)**phenyl**]-2-methylpyrimidine 20 starting from acetamidine and 1,3-bis (4-bromophenyl)propenone is reported. Compds. 5-7 and 17-20 all bind strongly to the minor groove of poly-dA•dT whereas 8,12 and 13 bind less tightly as judged by their  $\Delta T_m$  values. A similar trend was noted for binding of these compds. to the 12-mer-d(CGCGAATTCGCG)2. Compds. 5,7 and 17 are more active and less toxic than pentamidine at its ED when evaluated against *Pneumocystis carinii* pneumonia (PCP) in the immunosuppressed rat model.

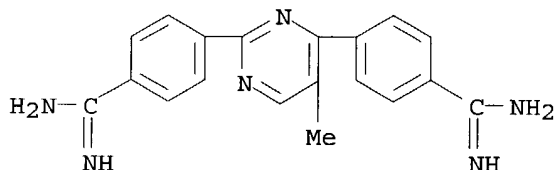
IT 160522-94-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(anti-pneumocystis *carinii* pneumonia activity of dicationic diaryl methylpyrimidines)

RN 160522-94-1 CAPLUS

CN Benzenecarboximidamide, 4,4'-(5-methyl-2,4-pyrimidinediyl)bis- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L11 ANSWER 34 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1998:21460 CAPLUS

DOCUMENT NUMBER: 128:121798

TITLE: Liquid crystal device and liquid crystal apparatus

INVENTOR(S): Tsuzuki, Hidetoshi; Kamio, Masaru; Okada, Shinjiro; Tsuboyama, Akira; Tokunaga, Hiroyuki; Tomono, Haruo; Sato, Koichi; Matsuo, Yuji; Katakura, Kazunori; Yokoyama, Yuko

PATENT ASSIGNEE(S): Canon Kabushiki Kaisha, Japan

SOURCE: Eur. Pat. Appl., 50 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 814142	A2	19971229	EP 1997-304210	19970616
EP 814142	A3	19981216		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 10068923	A2	19980310	JP 1997-153664	19970611
EP 1088877	A2	20010404	EP 2000-204626	19970616
EP 1088877	A3	20010411		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				



09/ 811,359

IE, FI

US 6252641 B1 20010626 US 1997-874458 19970617  
PRIORITY APPLN. INFO.: JP 1996-155503 A 19960617  
JP 1997-153664 A 19970611  
EP 1997-304210 A3 19970616

OTHER SOURCE(S): MARPAT 128:121798

AB A liquid crystal device is constituted by a pair of electrode plates and a liquid crystal composition disposed between the electrode plates. At least one of the electrode plates comprises a light-transmissive substrate, a plurality of electrodes including principal electrodes and auxiliary electrodes supported on the light-transmissive substrate, and an insulating layer. Each auxiliary electrode is disposed between an associated principal electrode and the light-transmissive substrate so as to be elec. connected with at least a part of the associated principal electrode, the auxiliary electrodes being disposed with spacings therebetween which are filled with the insulating layer. The liquid crystal composition comprises at least one species of a fluorine-containing mesomorphic compound comprising a fluorocarbon terminal portion and a hydrocarbon terminal portion, the terminal portions being connected with a central core and having smectic mesophase or latent smectic mesophase. The combination of the above specific cell structure and the specific liquid crystal composition is effective in improving display quality (e.g., contrast) while minimizing a voltage waveform deformation.

IT 173307-42-1

RL: TEM (Technical or engineered material use); USES (Uses)  
(liquid crystal composition for display devices)

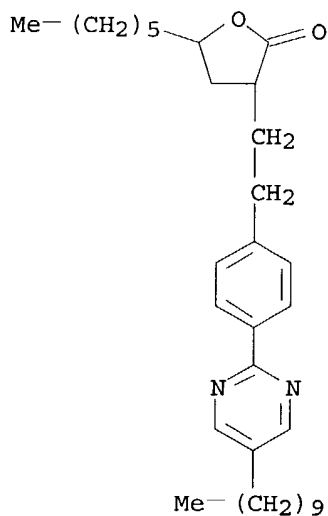
RN 173307-42-1 CAPLUS

CN 2(3H)-Furanone, 3-[2-[4-(5-decyl-2-pyrimidinyl)phenyl]ethyl]-5-hexyldihydro-, mixt. with 5-decyl-2-[4-[(2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctyl)oxy]phenyl]pyrimidine, 2-[4-[2,2-difluoro-2-[1,1,2,2-tetrafluoro-2-(nonafluorobutoxy)ethoxy]ethoxy]phenyl]-5-octylpyrimidine, 5-nonyl-2-[4-[(2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctyl)oxy]phenyl]pyrimidine and 5-octyl-2-[4-[(2,2,3,3,4,4,5,5,6,6,7,7,8,8,8-pentadecafluorooctyl)oxy]phenyl]pyrimidine (9CI) (CA INDEX NAME)

CM 1

CRN 170991-44-3

CMF C32 H48 N2 O2

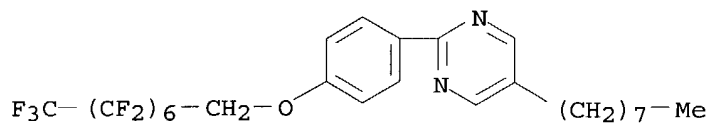


09/ 811,359

CM 2

CRN 152915-43-0

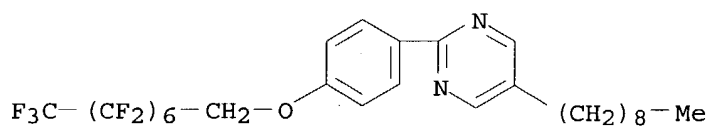
CMF C26 H25 F15 N2 O



CM 3

CRN 152915-42-9

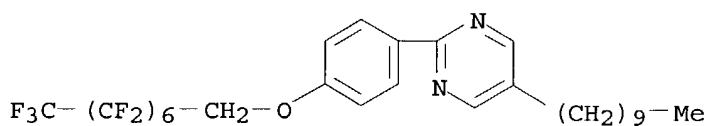
CMF C27 H27 F15 N2 O



CM 4

CRN 152915-41-8

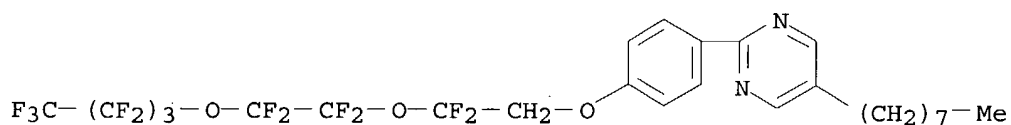
CMF C28 H29 F15 N2 O



CM 5

CRN 152914-98-2

CMF C26 H25 F15 N2 O3



L11 ANSWER 35 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:679042 CAPLUS

DOCUMENT NUMBER: 127:301549

TITLE: Preparation of liquid crystal compounds, liquid crystal compositions containing the compounds, and liquid crystal display devices made by using the compositions

09/ 811,359

INVENTOR(S): Ando, Tsugumichi; Matsui, Shuichi; Miyazawa, Kazutoshi; Takeuchi, Hiroyuki; Koizumi, Yasuyuki; Sekiguchi, Yasuko; Nakagawa, Etsuo; Takeshita, Fusayuki; et al.

PATENT ASSIGNEE(S): Chisso Corp., Japan; Ando, Tsugumichi; Matsui, Shuichi; Miyazawa, Kazutoshi; Takeuchi, Hiroyuki; Koizumi, Yasuyuki; Sekiguchi, Yasuko

SOURCE: PCT Int. Appl., 222 pp.  
CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

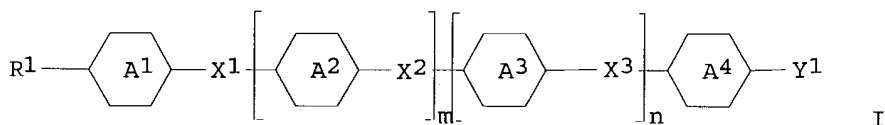
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9736847	A1	19971009	WO 1997-JP1048	19970327
W: AL, AU, BA, BB, BG, BR, CA, CN, CU, CZ, EE, GE, HU, IL, IS, JP, KR, LC, LK, LR, LT, LV, MG, MK, MN, MX, NO, NZ, PL, RO, SG, SI, SK, TR, TT, UA, US, UZ, VN, YU, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9720434	A1	19971022	AU 1997-20434	19970327
EP 916639	A1	19990519	EP 1997-908523	19970327
EP 916639	B1	20020612		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
CN 1218451	A	19990602	CN 1997-194642	19970327
CN 1118449	B	20030820		
EP 1043299	A2	20001011	EP 2000-113173	19970327
EP 1043299	A3	20040102		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, PT, IE				
JP 3231333	B2	20011119	JP 1997-535120	19970327
JP 2002053529	A2	20020219	JP 2001-181798	19970327
AT 219041	E	20020615	AT 1997-908523	19970327
TW 416979	B	20010101	TW 1997-86104142	19970328
US 6190576	B1	20010220	US 1998-155595	19980930
US 6319570	B1	20011120	US 2000-597280	20000619

PRIORITY APPLN. INFO.: JP 1996-79946 A 19960402  
JP 1996-239751 A 19960822  
EP 1997-908523 A3 19970327  
JP 1997-535120 A3 19970327  
WO 1997-JP1048 W 19970327  
US 1998-155595 A1 19980930

OTHER SOURCE(S): MARPAT 127:301549  
GI



AB The above liquid crystal compds. represented by general formula (I; R1, Y1 = C1-20 alkyl; X1, X2, X3 = a single bond, 1,2-ethylene, vinylene, CO2, CF2O or OCF2; A1, A2, A3, A4 = trans-1,4-cyclohexylene or optionally fluorinated or chlorinated 1,4-phenylene, at least one of A2, A3 and A4 being 2,3-difluoro-1,4-phenylene; m, n = 0 or 1) with the proviso that the elements constituting the compds. may be each replaced by isotopes thereof are prepared Liquid crystal compns. containing the compds. I and liquid crystal

display devices made by using the compns. are claimed. These liquid crystal compds. are low in viscosity and high in dielec. anisotropy and have high specific resistance and high voltage retention, and are stable even when exposed to heat and UV rays. Thus, 2,3-difluoro-4-ethoxyphenol was condensed with 2-fluoro-4-[2-(trans-4-propylcyclohexyl)ethyl]benzoic acid using DCC in the presence of 4-dimethylaminopyridine at room temperature overnight to give 2,3-difluoro-4-ethoxyphenyl 2-fluoro-4-[2-(trans-4-propylcyclohexyl)ethyl]benzoate (II), which showed phase transition temperature 65.4° for C-N point and 141.3° for N-I point. A liquid crystal composition containing 15 weight% II and a mother liquid crystal composition

(85

weight%) consisting of 4-butoxyphenyl 4-(trans-4-propylcyclohexyl)carboxybenzoate 27.6, 4-ethoxyphenyl 4-(trans-4-butylcyclohexyl)carboxybenzoate 20.7, 4-methoxyphenyl 4-(trans-4-pentylcyclohexyl)carboxybenzoate 20.7, 4-ethoxyphenyl 4-(trans-4-propylcyclohexyl)carboxybenzoate 17.2, and 4-ethoxyphenyl 4-(trans-4-pentylcyclohexyl)carboxybenzoate 13.8 weight% showed clearing point 129.4° and dielec. anisotropy ( $\Delta\epsilon$ ) -4.17 as compared to 74.6° and 0.0, resp., for the mother liquid crystal composition

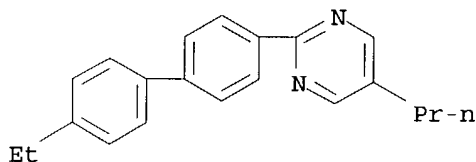
IT 175859-31-1

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(liquid crystal composition containing; preparation of liquid crystal compds., liquid crystal compns. containing the compds., and liquid crystal display devices made by using them)

RN 175859-31-1 CAPLUS

CN Pyrimidine, 2-(4'-ethyl[1,1'-biphenyl]-4-yl)-5-propyl- (9CI) (CA INDEX NAME)



L11 ANSWER 36 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:640630 CAPLUS

DOCUMENT NUMBER: 127:339303

TITLE: Bialkenyl derivatives, liquid crystalline compounds and liquid crystal compositions

INVENTOR(S): Kato, Takashi; Matsui, Shuichi; Miyazawa, Kazutoshi; Sekiguchi, Yasuko; Nakagawa, Etsuo

PATENT ASSIGNEE(S): Chisso Corp., Japan; Kato, Takashi; Matsui, Shuichi; Miyazawa, Kazutoshi; Sekiguchi, Yasuko; Nakagawa, Etsuo

SOURCE: PCT Int. Appl., 116 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9734855	A1	19970925	WO 1997-JP700	19970306
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IS, KE, KG, KR, KZ, LC, LK, LR,				

09/ 811,359

LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU,  
SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, AM, AZ,  
BY, KG, KZ, MD, RU, TJ, TM  
RW: GH, KE, LS, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FI, FR, GB,  
GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN,  
ML, MR, NE, SN, TD, TG

JP 10045639	A2	19980217	JP 1997-24331	19970123
AU 9722324	A1	19971010	AU 1997-22324	19970306
EP 891314	A1	19990120	EP 1997-905457	19970306
EP 891314	B1	20010905		

R: DE, FR, GB

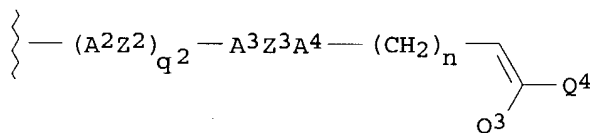
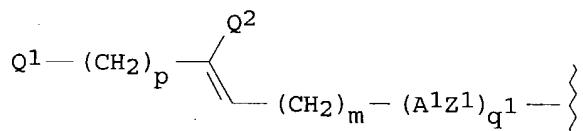
CN 1214036	A	19990414	CN 1997-193138	19970306
CN 1110470	B	20030604		
US 6180027	B1	20010130	US 1998-101990	19980722

PRIORITY APPLN. INFO.:

JP 1996-90585	A	19960318
WO 1997-JP700	W	19970306

OTHER SOURCE(S): MARPAT 127:339303

GI



I

AB Liquid crystalline compds. expressed by formula I (A1-4 = trans-1,4-cyclohexylene, etc.; Z1-3 = (CH2)2, etc.; Q1-2 = H, F, Cl, Br; Q3-4 = F, Cl, Br; m,n,p = integer 0-5; q1-q2 = integer 0-1), liquid crystal compns. thereof obtained by combination with specified liquid crystal compds., and liquid crystal display devices using them are disclosed. The compns. provide a wide liquid crystal phase temperature range.

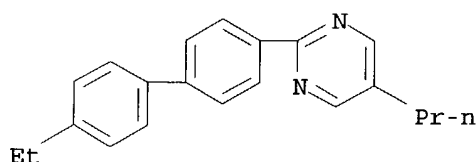
IT 175859-31-1

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(electrooptical display devices using liquid crystal compns. containing)

RN 175859-31-1 CAPLUS

CN Pyrimidine, 2-(4'-ethyl[1,1'-biphenyl]-4-yl)-5-propyl- (9CI) (CA INDEX NAME)



09/ 811,359

DOCUMENT NUMBER: 127:247916  
TITLE: Formylation of triflates by carbon monoxide and hydrosilanes  
INVENTOR(S): Kotsuki, Hikizo; Suenaga, Hitoshi; Datta, Peobal kanti  
PATENT ASSIGNEE(S): Teikoku Hormone Mfg. Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 09227439	A2	19970902	JP 1996-75107	19960222
PRIORITY APPLN. INFO.:			JP 1996-75107	19960222

OTHER SOURCE(S): CASREACT 127:247916

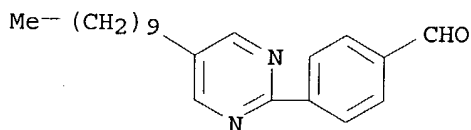
AB Triflates are formylated using CO as a C source and hydrosilanes as proton sources in the presence of catalysts. 4-Me<sub>3</sub>CC<sub>6</sub>H<sub>4</sub>O<sub>3</sub>SCF<sub>3</sub> was treated with CO in DMF in the presence of Pd(OAc)<sub>2</sub> and 1,3-bis(diphenylphosphino)propane at 70° for 20 min and treated with trioctylsilane and NEt<sub>3</sub> at 70° to give 89% 4-Me<sub>3</sub>CC<sub>6</sub>H<sub>4</sub>CHO.

IT 177581-96-3P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)  
(formylation of triflates by CO and hydrosilanes)

RN 177581-96-3 CAPLUS

CN Benzaldehyde, 4-(5-decyl-2-pyrimidinyl)- (9CI) (CA INDEX NAME)



L11 ANSWER 38 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:299249 CAPLUS

DOCUMENT NUMBER: 126:285791

TITLE: Liquid crystalline compound substituted with fluorine containing group, liquid crystal composition, and liquid crystal display device

INVENTOR(S): Miyazawa, Kazutoshi; Matsui, Shuichi; Kondo, Tomoyuki; Kato, Takashi; Sekiguchi, Yasuko; Nakagawa, Etsuo

PATENT ASSIGNEE(S): Chisso Corp., Japan

SOURCE: Eur. Pat. Appl., 58 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

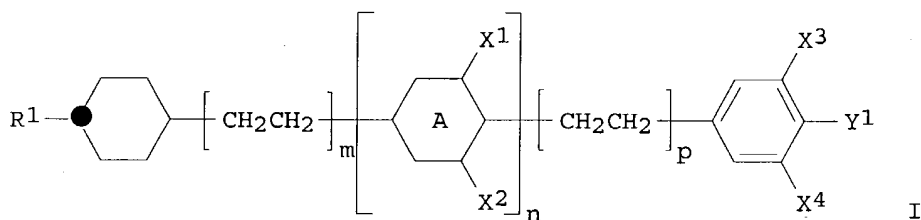
FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 761799	A1	19970312	EP 1996-113195	19960816
R: CH, DE, FR, GB, LI				
JP 09137162	A2	19970527	JP 1995-319515	19951114
JP 09137163	A2	19970527	JP 1995-319516	19951114
JP 09137164	A2	19970527	JP 1995-319517	19951114
JP 2896648	B2	19990531		
TW 426723	B	20010321	TW 1996-85107358	19960618

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US 5948318 A 19990907 US 1996-698456 19960815  
US 6117360 A 20000912 US 1996-698451 19960815  
CN 1153807 A 19970709 CN 1996-111984 19960910  
PRIORITY APPLN. INFO.: JP 1995-258185 A 19950911  
JP 1995-319517 A 19951114  
OTHER SOURCE(S): MARPAT 126:285791  
GI

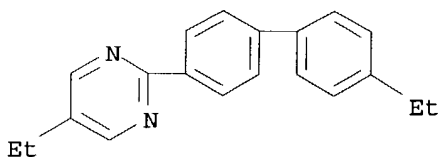


AB The liquid crystalline compds. I are given wherein R1 represents an alkyl group having 1-10 C atoms, ring A represents 1,4-phenylene or 1,4-cyclohexylene, each of X1, X2, X3, and X4 independently represents H atom or F atom, Y1 represents CF3 or OCF3, and each of m, n, and p is independently an integer of 1 or 0. The liquid crystalline compds. have a wide temperature range of nematic phase, low viscosity, large pos.  $\Delta\epsilon$ , high chemical stability, high miscibility with other liquid crystalline compds. at low temps., small temperature dependency of viscosity and  $\Delta\epsilon$ , extremely high specific resistance (high voltage holding ratio), and good UV stability, and are preferably used for TFT. Also, disclosed are liquid crystal compns. containing the liquid crystalline compds. mentioned above, and liquid crystal display devices using the liquid crystal composition

IT **148832-61-5D**, mixture containing  
RL: TEM (Technical or engineered material use); USES (Uses)  
(liquid crystal)

RN 148832-61-5 CAPLUS

CN Pyrimidine, 5-ethyl-2-(4'-ethyl[1,1'-biphenyl]-4-yl)- (9CI) (CA INDEX NAME)



L11 ANSWER 39 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1997:51535 CAPLUS

DOCUMENT NUMBER: 126:74854

TITLE: Preparation of arylazolones as agrochemical fungicides.

INVENTOR(S): Brown, Richard James; Sun, King-Mo; Frasier, Deborah Ann

PATENT ASSIGNEE(S): E. I. Du Pont de Nemours & Co., USA; Brown, Richard James; Sun, King-Mo; Frasier, Deborah Ann

SOURCE: PCT Int. Appl., 95 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

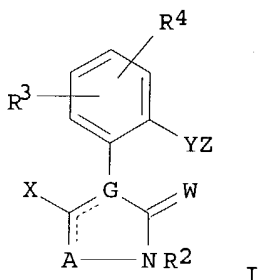
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

09/ 811,359

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9636615	A1	19961121	WO 1995-US5847	19950516
W: JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 10504042	T2	19980414	JP 1995-534772	19950516
PRIORITY APPLN. INFO.:			WO 1995-US5847	19950516
OTHER SOURCE(S):			MARPAT 126:74854	
GI				



AB Title compds. [I; A = O, S, N, NR5, CR14; G = C, N; W = O, S; X = OR1, SR1, SOR1, SO2R1, halo; R1 = alkyl, haloalkyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl, cycloalkyl, alkylcarbonyl, alkoxycarbonyl, (substituted) PhCO; R2, R5 = H, R1; R3, R4 = H, halo, cyano, NO2, alkyl, haloalkyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl, alkoxy, haloalkoxy, alkenyloxy, alkynyloxy; Y O, S, SO, SO2, CHR6O, CHR6ON:CR7, C.tplbond.C, bond, etc.; R6 = H, alkyl; R7 = H, alkyl, haloalkyl, alkoxy, haloalkoxy, alkenyl, haloalkenyl, alkynyl, haloalkynyl, cycloalkyl, alkylcarbonyl, alkoxycarbonyl, cyano, morpholino; R14 = H, halo, alkyl, haloalkyl, alkenyl, haloalkenyl, alkynyl, haloalkynyl, cycloalkyl; Z = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, Ph, (aromatic) heterocyclyl, etc.; with provisos], were prepared Thus, o-tolyl isocyanate reacted with Me2NNH2 in PhMe to give 2,2-dimethyl-N-(2-methylphenyl)hydrazinecarboxamide. This was refluxed with triphosgene in CH2Cl2 to give 5-chloro-2,4-dihydro-2-methyl-4-(2-methylphenyl)-3H-1,2,4-triazol-3-one, which was converted to 2,4-dihydro-5-methoxy-2-methyl-4-[2-[[[(phenylmethylene)amine]oxy]methyl]phenyl]-3H-1,2,4-triazol-3-one. Several title compds. gave complete control of Erysiphe graminis, Puccinia recondita, and Plasmopara viticola.

IT 185336-64-5P

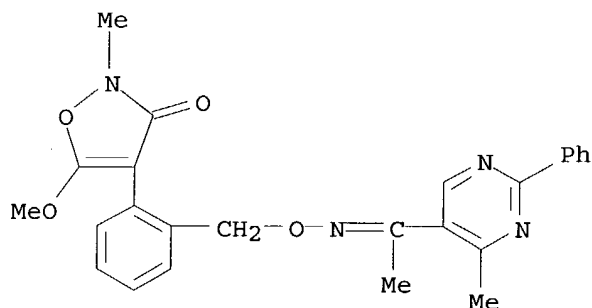
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of arylazolones as agrochem. fungicides)

RN 185336-64-5 CAPLUS

CN 3(2H)-Isoxazolone, 5-methoxy-2-methyl-4-[2-[[[1-(4-methyl-2-phenyl-5-pyrimidinyl)ethylidene]amino]oxy]methyl]phenyl]- (9CI) (CA INDEX NAME)



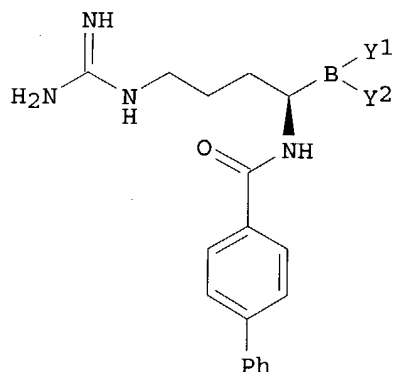
09/ 811,359



L11 ANSWER 40 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1996:672852 CAPLUS  
DOCUMENT NUMBER: 126:31466  
TITLE: Boronic acid and ester inhibitors of thrombin  
INVENTOR(S): Amparo, Eugene C.; Miller, William H.; Pacofsky, Gregory J.; Wityak, John; Weber, Patricia C.; Duncia, John J. V.; Santella, Joseph B., III  
PATENT ASSIGNEE(S): The Dupont Merck Pharmaceutical Company, USA  
SOURCE: U.S., 170 pp., Cont.-in-part of U.S. Ser. No. 348,029.  
CODEN: USXXAM  
DOCUMENT TYPE: Patent  
LANGUAGE: English  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5563127 A		19961008	US 1994-364338	19941227
PRIORITY APPLN. INFO.:			US 1993-36377	19930324
			US 1994-318029	19941004
			US 1994-348029	19941201

OTHER SOURCE(S): MARPAT 126:31466  
GI



AB Novel boronic acid and ester and carboxyl-modified amino acid compds.  
R1-Z-CHR2-A (A = organoboryl, BY1Y2; Y1, Y2 = independently OH, F, organoamino, C1-8 alkoxy, Y1Y2 = cyclic boron ester, amide containing N, S, O; etc.; Z = (CH2)mCX, X = amido, thioamido, etc., substituted C1-12 alkyl, alkenyl, etc.; R1 = arylalkenyl, aryl = substituted Ph, **naphthyl**, biphenyl, etc.; R2 = substituted C1-12 alkyl, alkenyl, etc.), which are inhibitors of trypsin-like enzymes, are disclosed. Thus, amino acid modified boronic ester I (Y1Y2 = (+)-pinanediol) was prepared in multiple

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steps starting from (+)-pinanediol 4-bromo-1(R)-(4-phenylbenzoyl)aminobutane-1-boronate. Thrombin inhibition activity of some of the compds. prepared is described.

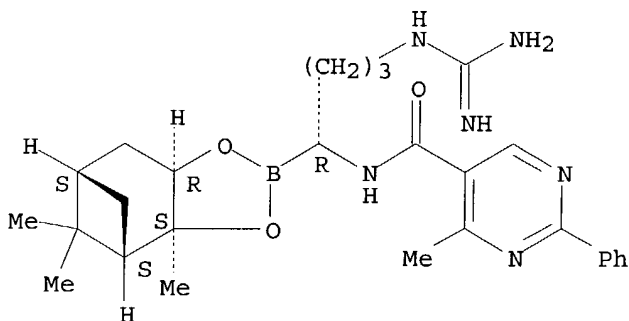
IT 180896-93-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)  
(preparation of amino acid-modified boronic acids and esters as inhibitors of thrombin)

RN 180896-93-9 CAPLUS

CN 5-Pyrimidinecarboxamide, N-[(1R)-4-[(aminoiminomethyl)amino]-1-[(3aS,4S,6S,7aR)-hexahydro-3a,5,5-trimethyl-4,6-methano-1,3,2-benzodioxaborol-2-yl]butyl]-4-methyl-2-phenyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 41 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:466907 CAPLUS

DOCUMENT NUMBER: 125:127905

TITLE: Ethynylene compound for liquid-crystal composition and liquid-crystal display element using same

INVENTOR(S): Takiguchi, Takao; Iwaki, Takashi; Tokano, Goji; Yamada, Yoko; Nakamura, Shinichi

PATENT ASSIGNEE(S): Canon Kk, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 35 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08109145	A2	19960430	JP 1994-271847	19941012

PRIORITY APPLN. INFO.: JP 1994-271847 19941012

AB Claimed is an ethynylene compound such as 1-(5-decyloxy-pyrimidine-2-yl)-4-(4-phenyl-1-butynyl)benzene. A liquid-crystal composition contains an ethynylene compound, and a liquid-crystal display element comprises the above liquid-crystal composition layer enclosed between a pair of electrode substrates.

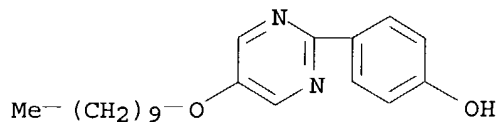
IT 110203-06-0

RL: RCT (Reactant); RACT (Reactant or reagent)  
(ethynylene compound for liquid-crystal composition from)

RN 110203-06-0 CAPLUS

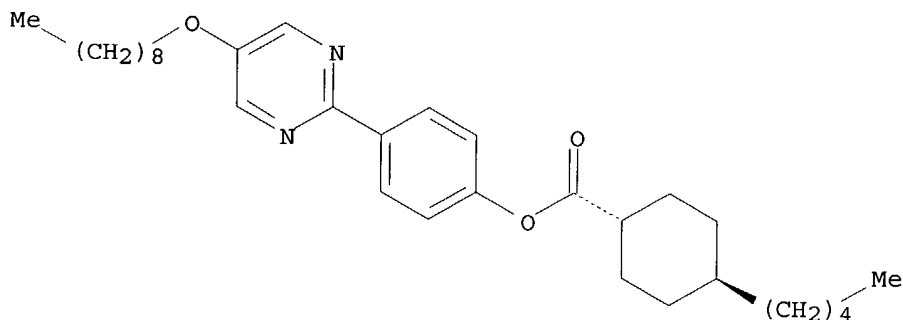
CN Phenol, 4-[5-(decyloxy)-2-pyrimidinyl]- (9CI) (CA INDEX NAME)

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L11 ANSWER 42 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1996:353352 CAPLUS  
DOCUMENT NUMBER: 124:356726  
TITLE: Synthesis and mesomorphic properties of fluorinated liquid crystals obtained from optically active 2-fluoro-octanol  
AUTHOR(S): Liu, Hong; Nohira, Hiroyuki  
CORPORATE SOURCE: Dep. Applied Chem., Saitama Univ., Urawa, 338, Japan  
SOURCE: Liquid Crystals (1996), 20(5), 581-586  
CODEN: LICRE6; ISSN: 0267-8292  
PUBLISHER: Taylor & Francis  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Several homologs of semi-fluorinated liquid crystals, 4'-[(n-perfluoroalkyl)alkyloxy]phenyl 4-(2-fluorooctyloxy)benzoates and 4'-(2-fluorooctyloxy)phenyl 4-[(n-perfluoroalkyl)alkyloxy]benzoates were synthesized. One set of the compds., with the central carbonyl group conjugated to the terminal position carrying the nonchiral perfluoroalkyloxy tail, showed enhanced chiral smectic C behavior, while the other set, with the central carbonyl group conjugated to the terminal position carrying the chiral 2-fluoro-octyloxy tail, exhibited enhanced smectic A behavior. The mesomorphic properties of these novel fluorinated materials are reported and the effects of extent of fluorination are discussed.  
IT 122893-54-3  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)  
(liquid crystal properties of phenylpyrimidine mixture doped with (fluorooctyl) (perfluoroalkylalkoxy) benzenes)  
RN 122893-54-3 CAPLUS  
CN Cyclohexanecarboxylic acid, 4-pentyl-, 4-[5-(nonyloxy)-2-pyrimidinyl]phenyl ester, trans- (9CI) (CA INDEX NAME)

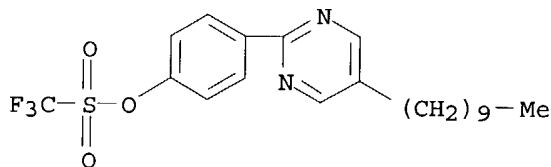
Relative stereochemistry.



L11 ANSWER 43 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1996:253101 CAPLUS  
DOCUMENT NUMBER: 125:32885  
TITLE: An efficient procedure for palladium-catalyzed hydroformylation of aryl/enol triflates

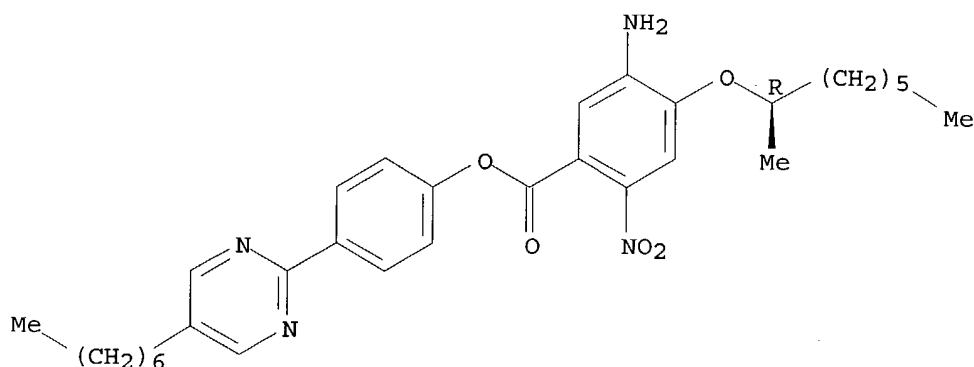
09/ 811,359

AUTHOR(S): Kotsuki, Hiyoshizo; Datta, Probal Kanti; Suenaga, Hitoshi  
CORPORATE SOURCE: Faculty Science, Kochi Univ., Kochi, 780, Japan  
SOURCE: Synthesis (1996), (4), 470-2  
CODEN: SYNTBF; ISSN: 0039-7881  
PUBLISHER: Thieme  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
OTHER SOURCE(S): CASREACT 125:32885  
AB An efficient method for hydroformylation of aryl and enol trifluoromethanesulfonates is presented. Their reaction with CO, trioctylsilane, and Et<sub>3</sub>N in the presence of a catalytic amount of Pd(OAc)<sub>2</sub> and 1,3-bis(diphenylphosphanyl)propane proceeds efficiently to provide a variety of aromatic and  $\alpha,\beta$ -unsatd. aldehydes.  
IT 173346-92-4  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(preparation of aromatic and  $\alpha,\beta$ -unsatd. aldehydes by palladium-catalyzed hydroformylation of aryl/enol triflates)  
RN 173346-92-4 CAPLUS  
CN Methanesulfonic acid, trifluoro-, 4-(5-decyl-2-pyrimidinyl)phenyl ester (9CI) (CA INDEX NAME)



L11 ANSWER 44 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1996:192841 CAPLUS  
DOCUMENT NUMBER: 124:290393  
TITLE: The synthesis of nitroaniline monomers and polymers as non-linear optical ferroelectric liquid crystals  
AUTHOR(S): Chen, X. H.; Herr, R. P.; Schmitt, K.; Buchecker, R.  
CORPORATE SOURCE: Dep. RLCR, F. Hoffmann-La Roche Ltd., Basel, 4002, Switz.  
SOURCE: Liquid Crystals (1996), 20(2), 125-38  
CODEN: LICRE6; ISSN: 0267-8292  
PUBLISHER: Taylor & Francis  
DOCUMENT TYPE: Journal  
LANGUAGE: English  
AB Chiral 2-amino-4-alkoxy-5-nitrobenzoate and 5-amino-4-alkoxy-2-nitrobenzoate derivs. as well as the corresponding biphenyl derivs. were synthesized. Some of them were also derivatized to the corresponding acrylates and polyacrylates. Many of the new substances exhibit a large spontaneous polarization and large second-order NLO coeffs. In addition some of them show a broad range SC\* phase. All these properties depend strongly on small changes in the mol. structures. Here we present the synthesis of these novel NLO FLC materials and discuss some of their properties.  
IT 147970-12-5  
RL: PRP (Properties)  
(nitroaniline monomers and polymers as nonlinear optical ferroelec. liquid crystals)  
RN 147970-12-5 CAPLUS  
CN Benzoic acid, 5-amino-4-[(1-methylheptyl)oxy]-2-nitro-, 4-(5-heptyl-2-pyrimidinyl)phenyl ester, (R)- (9CI) (CA INDEX NAME)

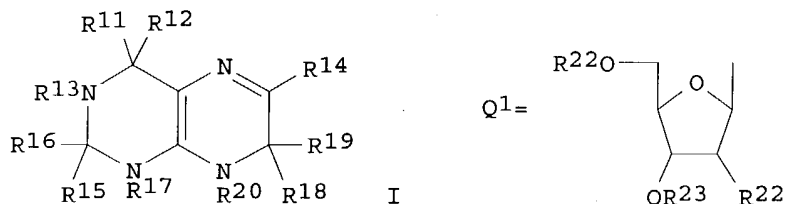
Absolute stereochemistry.



L11 ANSWER 45 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1996:170748 CAPLUS  
 DOCUMENT NUMBER: 124:261618  
 TITLE: Preparation of pteridine nucleotide analogs as  
 fluorescent DNA probes.  
 INVENTOR(S): Hawkins, Mary E.; Pfleiderer, Wolfgang; Davis, Michael  
 Dean; Balis, Frank  
 PATENT ASSIGNEE(S): United States Dept. of Health and Human Services, USA  
 SOURCE: PCT Int. Appl., 103 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9531469	A1	19951123	WO 1995-US5264	19950425
W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IS, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TT				
RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5525711	A	19960611	US 1994-245923	19940518
CA 2190588	AA	19951123	CA 1995-2190588	19950425
CA 2190588	C	20030318		
AU 9523991	A1	19951205	AU 1995-23991	19950425
AU 688036	B2	19980305		
EP 759927	A1	19970305	EP 1995-917197	19950425
EP 759927	B1	19980624		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
JP 10500949	T2	19980127	JP 1995-529675	19950425
AT 167680	E	19980715	AT 1995-917197	19950425
ES 2118593	T3	19980916	ES 1995-917197	19950425
US 5612468	A	19970318	US 1995-451641	19950526
PRIORITY APPLN. INFO.:				
			US 1994-245923	A 19940518
			WO 1995-US5264	W 19950425
OTHER SOURCE(S): MARPAT 124:261618				
GI				

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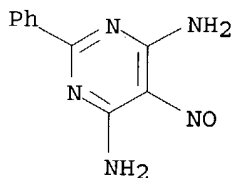


AB Title compds. [I; R11R12 = O, or R11R13 = bond; R12 = (protected) NH<sub>2</sub>; R13 = H, alkyl; R14 = H, alkyl, Ph; R15R16 = O, or R15R17 = bond; R16 = H, Ph, (protected) NH<sub>2</sub>; R18R19 = O; R18R20 = bond; R17, R20 = Q1; R21 = H, triphosphate, protecting group; R22 = H, (protected) OH; R23 = H, phosphoramidite, phosphonate, methylphosphonate, phosphorothioate, phosphotriester, hemisuccinate (bound to a solid support), carbodiimide (bound to a solid support); with provisos], were prepared Thus, 4-amino-6-phenyl-8-(5-O-dimethoxytrityl-2-deoxy-β-D-ribofuranosyl)pteridine-7-one 3'-O-(β-cyanoethyl, N-diisopropyl)phosphoramidite was prepared via 4-amino-6-phenylpteridine-7-one and used in a double-stranded DNA segment for realtime determination of HIV-1 integrase activity.

IT **56472-04-9P**, 2-Phenyl-4,6-diamino-5-nitrosopyrimidine  
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)  
 (preparation of pteridine nucleotide analogs as fluorescent DNA probes)

RN 56472-04-9 CAPLUS

CN 4,6-Pyrimidinediamine, 5-nitroso-2-phenyl- (9CI) (CA INDEX NAME)



L11 ANSWER 46 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1996:137584 CAPLUS

DOCUMENT NUMBER: 124:176140

TITLE: Preparation of optically active heteroarylalkanol and arylalkanol

INVENTOR(S): Azumai, Takayuki; Minamii, Masayoshi; Fujimoto, Yukari; Matsumoto, Tsutomu

PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.  
 CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07291940	A2	19951107	JP 1994-89663	19940427
JP 3486685	B2	20040113		

PRIORITY APPLN. INFO.: JP 1994-89663 19940427

OTHER SOURCE(S): CASREACT 124:176140; MARPAT 124:176140

GI

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The title compound represented by formula  $R_1(O)mA_1(A_2)pA_3(CH_2)nR$  [I; R = CH(OH)Me;  $R_1$  = C1-20 (halo)alkyl, C2-20 (halo)alkoxyalkyl;  $A_1$ ,  $A_2$ ,  $A_3$  = Q - Q9; wherein u, w = 0-3; provided that when  $A_1$  = fused ring,  $A_2$  = monocyclic ring or when  $A_1$  = monocyclic ring and p = 1,  $A_2$  and  $A_3$  = monocyclic ring; n = 0-10; m, p = 0,1], useful as an intermediate for agrochems., drugs and ferroelec. liquid crystals, is prepared by hydrosilylation of an  $\alpha$ -alkene I (R = CH:CH<sub>2</sub>) with HSi(X<sub>5</sub>)<sub>3</sub> (X<sub>5</sub> = H, alkyl, alkoxy, halo) in the presence of a transition metal complex having an optically active tert-phosphine binaphthyl compound [R<sub>2</sub> = halo, alkoxy, alkoxyalkoxy, (phenyl)alkyl, C5-7 cycloalkyl; R<sub>3</sub> = alkyl, alkoxy, (halo)phenyl; R<sub>4</sub>, R<sub>5</sub> = H, alkyl; or R<sub>4</sub>R<sub>5</sub> forms a fused ring] and oxidation of the resulting silane I [R = CHMeSi(X<sub>5</sub>)<sub>3</sub>]. Thus, 5.4 g trichlorosilane was slowly added dropwise to a mixture of 10 g 2-[4-(5-hexen-1-yl)phenyl]-5-octyloxy-pyrimidine, 0.46 mg  $\pi$ -allylpalladium chloride, and 1.22 mg (S)-I (R<sub>2</sub> = Me, R<sub>3</sub> = Ph, R<sub>4</sub> = R<sub>5</sub> = H) at 25-30° and the resulting mixture was stirred for 10 h and added to a suspension of 1.7 g KF and 9 g KHCO<sub>3</sub> in 100 mL THF and 100 mL MeOH under ice-cooling. The resulting mixture was stirred under ice-cooling for 2 h, followed by adding 25 mL 30% H<sub>2</sub>O<sub>2</sub>, and the reaction mixture was stirred at 50° for 24 h to give, after silica gel chromatog., the optically active title compound [(*-*)-II].

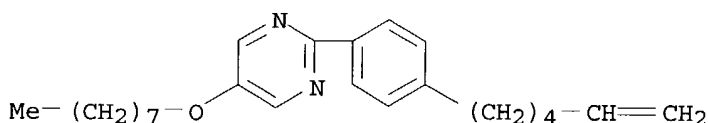
IT 165320-52-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of optically active heteroarylalkanol and arylalkanol by hydrosilylation of heteroaryl- or aryl- $\alpha$ -alkene with trichlorosilane)

RN 165320-52-5 CAPLUS

CN Pyrimidine, 2-[4-(5-hexenyl)phenyl]-5-(octyloxy)- (9CI) (CA INDEX NAME)



L11 ANSWER 47 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:950790 CAPLUS

DOCUMENT NUMBER: 124:144907

TITLE: An efficient procedure for palladium-catalyzed reduction of aryl/enol triflates

AUTHOR(S): Kotsuki, Hiyoshizo; Datta, Probal Kanti; Hayakawa, Hiroyuki; Suenaga, Hitoshi

CORPORATE SOURCE: Dep. of Chemistry, Kochi Univ., Kochi, 780, Japan

SOURCE: Synthesis (1995), (11), 1348-50

CODEN: SYNTBF; ISSN: 0039-7881

PUBLISHER: Thieme

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:144907

AB An efficient procedure to deoxygenate phenols and enols via trifluoromethanesulfonates is presented. Their reduction with Et<sub>3</sub>SiH in the presence of a catalytic amount of Pd(OAc)<sub>2</sub> and bidentate phosphine ligands such as 1,3-bis(diphenylphosphino)propane or 1,1'-bis(diphenylphosphino)ferrocene proceeded efficiently to afford a variety

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of aromatic, heteroarom., and olefinic compds.

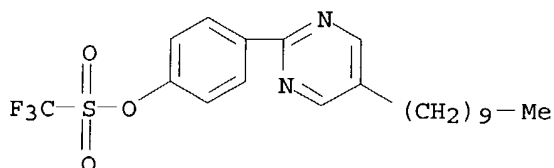
IT 173346-92-4

RL: RCT (Reactant); RACT (Reactant or reagent)

(palladium-catalyzed reduction of aryl enol triflates with triethylsilane)

RN 173346-92-4 CAPLUS

CN Methanesulfonic acid, trifluoro-, 4-(5-decyl-2-pyrimidinyl)phenyl ester  
(9CI) (CA INDEX NAME)



L11 ANSWER 48 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:604529 CAPLUS

DOCUMENT NUMBER: 123:156562

TITLE: Phenyl ester compound, its manufacture, and  
ferroelectric liquid-crystal mixture containing the  
compound

INVENTOR(S): Ishizuka, Hidemi; Nishama, Isa; Yokoyama, Akihisa

PATENT ASSIGNEE(S): Japan Enajii Kk, Japan

SOURCE: Jpn. Kokai Tokyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

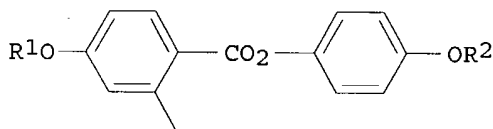
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07089904	A2	19950404	JP 1993-233272	19930920
PRIORITY APPLN. INFO.:			JP 1993-233272	19930920
OTHER SOURCE(S):		MARPAT 123:156562		

GI



II

AB The Ph ester is QOCOCH2CHMe(CH2)2CO2Q (I; R1-2 = C1-15 alkyl). I may be optically active QOCOCH2C\*HMe(CH2)2CO2Q (Q=II). The mixture contains  $\geq 1$  I. I is manufactured by esterification of 2 equivalent 5-alkyloxy-2-(4-alkyloxyphenoxy)carbonylphenol QOH and 1 equivalent XOC(CH2)2CHMeCH2COX (X = OH, halo). The compound is useful to control cholesteric pitches of ferroelec. liquid-crystal mixts. for electrooptical elements.

IT 166522-78-7

RL: TEM (Technical or engineered material use); USES (Uses)

(ferroelec. liquid-crystal mixture containing optically active Ph ester)

RN 166522-78-7 CAPLUS

CN Hexanedioic acid, 3-methyl-, bis[5-(octyloxy)-2-[[4-(octyloxy)phenoxy]carbonyl]phenyl] ester, (R)-, mixt. with  
2-[4-(decyloxy)phenyl]-5-octylpyrimidine, 2-[4-(hexyloxy)phenyl]-5-



09/ 811,359

nonylpyrimidine, 2-[4-(hexyloxy)phenyl]-5-octylpyrimidine and  
2-[4-(nonyloxy)phenyl]-5-octylpyrimidine (9CI) (CA INDEX NAME)

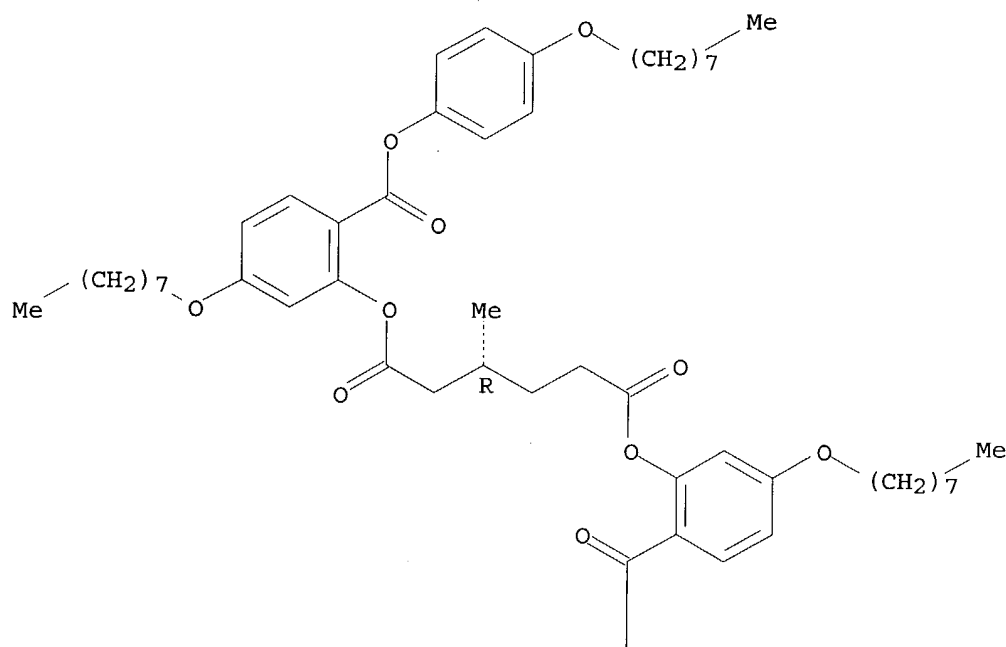
CM 1

CRN 165686-74-8

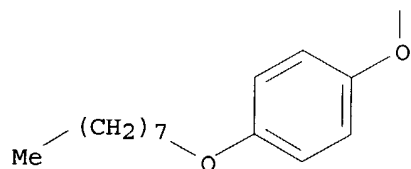
CMF C65 H92 O12

Absolute stereochemistry.

PAGE 1-A



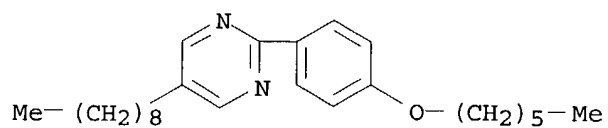
PAGE 2-A



CM 2

CRN 57202-56-9

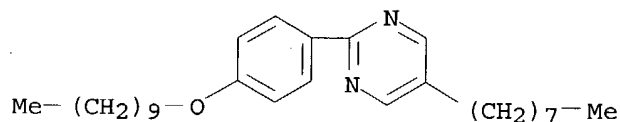
CMF C25 H38 N2 O



09/ 811,359

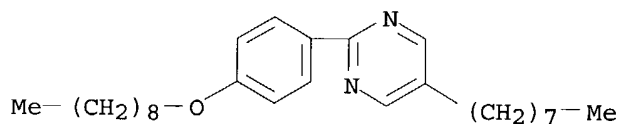
CM 3

CRN 57202-52-5  
CMF C28 H44 N2 O



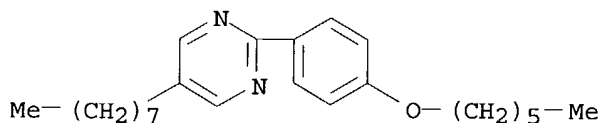
CM 4

CRN 57202-51-4  
CMF C27 H42 N2 O



CM 5

CRN 57202-48-9  
CMF C24 H36 N2 O



L11 ANSWER 49 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:576985 CAPLUS

DOCUMENT NUMBER: 123:98128

TITLE: Phenyl benzoate derivative optically active compound, liquid-crystal composition containing it, and phenolic derivative intermediate  
INVENTOR(S): Kobayashi, Shogo; Ishibashi, Shigeki; Horie, Toshio; Tsuru, Shinji; Nakamura, Kozaburo; Maruno, Tooru  
PATENT ASSIGNEE(S): Nippon Telegraph & Telephone, Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07069990	A2	19950314	JP 1994-136138	19940617
JP 07121892	B4	19951225		

09/ 811,359

PRIORITY APPLN. INFO.:

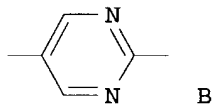
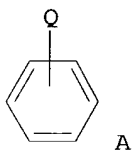
JP 1994-136138

19940617

OTHER SOURCE(S):

MARPAT 123:98128

GI



AB The compound is a Ph benzoate derivative I [W = R1XC02; R1 = C4-22 alkyl, C4-22 alkoxy; X = 1,4-C6H4, A, (1,4-C6H4)2, A-1,4-C6H4, 1,4-C6H4-1,4-C6H8, A-1,4-C6H8, B-1,4-C6H4; Q = halo, NO2, OH; Y = halo, Me, NO2; Z = Me, halo, CF3; R2 = C≤10 alkyl, alkoxy, aryl, aralkyl; C\* = optically active C; m = 0, 1; n = 0-6]. The composition contains ≥1 I. The intermediate for the optically active compound is I (W = OH). The compound showed large self polarization and the composition showed high response to be useful for optical display devices.

IT 165538-96-5

RL: TEM (Technical or engineered material use); USES (Uses)

(Ph benzoate derivative optically active compound and ferroelec. liquid-crystal composition containing it and its intermediate)

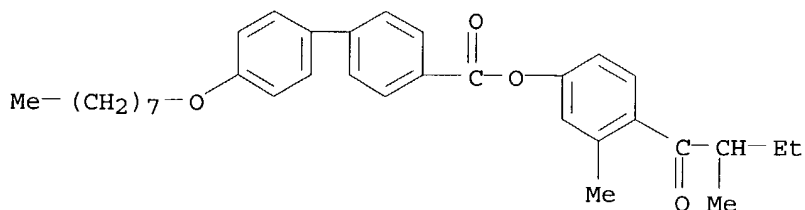
RN 165538-96-5 CAPLUS

CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-(octyloxy)-, 3-methyl-4-(2-methyl-1-oxobutyl)phenyl ester, mixt. with 5-(heptyloxy)-2-[4-(nonyloxy)phenyl]pyrimidine, 2-[4-(hexyloxy)phenyl]-5-(octyloxy)pyrimidine and 5-(octyloxy)-2-[4-(octyloxy)phenyl]pyrimidine (9CI) (CA INDEX NAME)

CM 1

CRN 123020-69-9

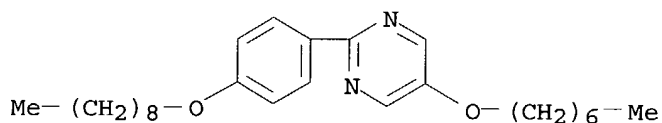
CMF C33 H40 O4



CM 2

CRN 121554-50-5

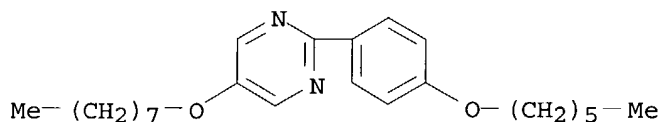
CMF C26 H40 N2 O2



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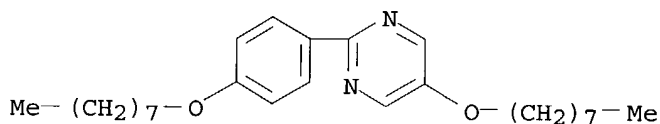
CM 3

CRN 120091-49-8  
CMF C24 H36 N2 O2



CM 4

CRN 114767-84-9  
CMF C26 H40 N2 O2



L11 ANSWER 50 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:513318 CAPLUS

DOCUMENT NUMBER: 123:71030

TITLE: Heterotrimeric liquid crystalline thiadiazole derivatives

AUTHOR(S): Zab, Kerstin; Joachimi, Detlev; Novotna, Eva; Diele, Siegmund; Tschierske, Carsten

CORPORATE SOURCE: Dep. Chem., Martin-Luther-Univ., Saale, Weinbergweg, D-06015/16, Germany

SOURCE: Liquid Crystals (1995), 18(4), 631-7

CODEN: LICRE6; ISSN: 0267-8292

PUBLISHER: Taylor & Francis

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Various trimeric cooligomers combining 2-phenyl-1,3,4-thiadiazole mesogenic moieties with a biphenyl mesogenic moiety were synthesized and their mesomorphic behavior studied by polarizing microscopy, calorimetry and x-ray scattering. Such cooligomeric structures provide an opportunity to combine different mesogenic units. Thus readily accessible homochiral biphenyl mesogenic units were connected with thiadiazole mesogenic units leading to an oligomeric liquid crystal material with ferroelec. properties.

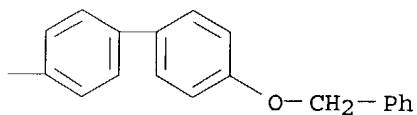
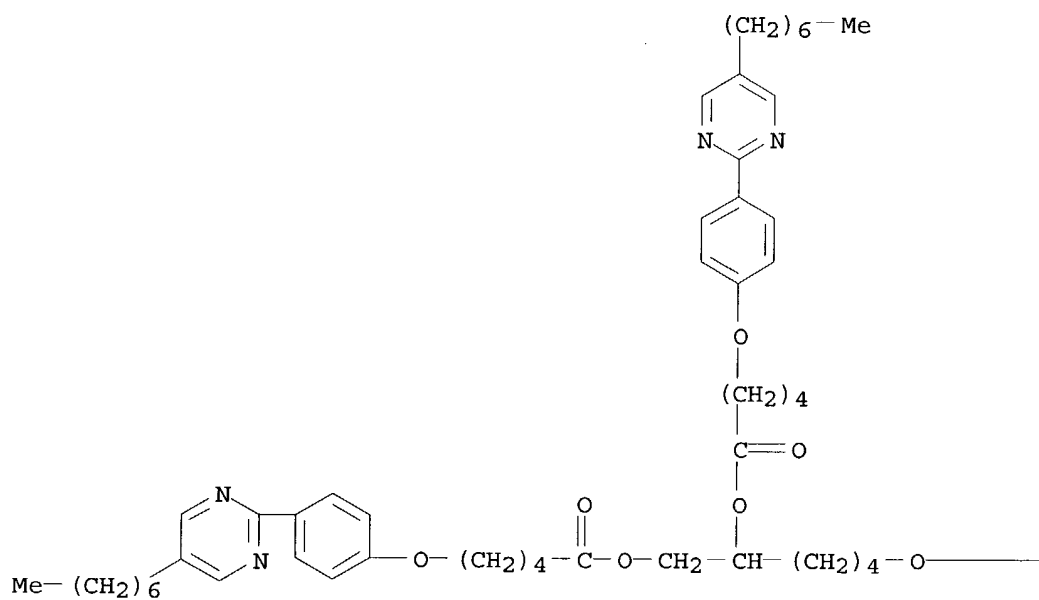
IT 164667-82-7P

RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(preparation and ferroelec. and liquid crystal properties of)

RN 164667-82-7 CAPLUS

CN Pentanoic acid, 5-[4-(5-heptyl-2-pyrimidinyl)phenoxy]-, 1-[4-[[4'-(phenylmethoxy)[1,1'-biphenyl]-4-yl]oxy]butyl]-1,2-ethanediyl ester (9CI) (CA INDEX NAME)



L11 ANSWER 51 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1995:489324 CAPLUS  
 DOCUMENT NUMBER: 123:22735  
 TITLE: Trimeric and tetrameric liquid crystalline thiadiazole derivatives  
 AUTHOR(S): Zab, K.; Joachimi, D.; Agert, O.; Neumann, B.; Tschierske, C.  
 CORPORATE SOURCE: Inst. Org. Chem., Martin-Luther-Univ.

09/ 811,359

SOURCE: Halle-Wittenberg, Halle/Saale, D-06015, Germany  
Liquid Crystals (1995), 18(3), 489-94  
CODEN: LICRE6; ISSN: 0267-8292

PUBLISHER: Taylor & Francis

DOCUMENT TYPE: Journal

LANGUAGE: English

AB Novel liquid crystalline 2-phenyl-1,3,4-thiadiazole based oligomers with three and four rigid aromatic units linked by a flexible central unit were studied by polarizing microscopy. The synthesis of these compds. and the influence of structural variations on the mesomorphic properties are described. The combination of suitable mesogenic moieties with appropriate central units leads to oligomers which exhibit SC phases.

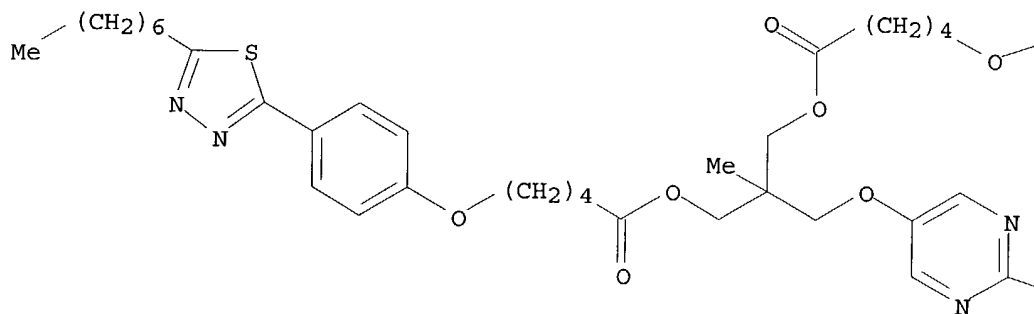
IT 164074-96-8P  
RL: PEP (Physical, engineering or chemical process); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)  
(preparation and liquid crystals properties of)

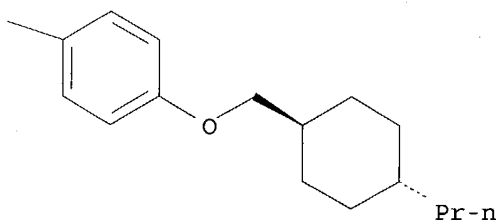
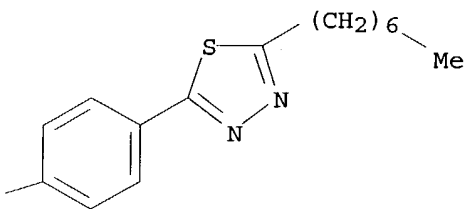
RN 164074-96-8 CAPLUS

CN Pentanoic acid, 5-[4-(5-heptyl-1,3,4-thiadiazol-2-yl)phenoxy]-, 2-methyl-2-[[[2-[4-[(4-propylcyclohexyl)methoxy]phenyl]-5-pyrimidinyl]oxy]methyl]-1,3-propanediyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A





L11 ANSWER 52 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:207982 CAPLUS

DOCUMENT NUMBER: 122:93024

TITLE: Perfluoroalkyloxyphenyl fluoroalkyloxybenzoate, its preparation, its-containing liquid crystal composition, and display

INVENTOR(S): Nohira, Hiroyuki; Sakaigawa, Akira

PATENT ASSIGNEE(S): Idemitsu Petrochemical Co, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06239802	A2	19940830	JP 1993-46113	19930212
PRIORITY APPLN. INFO.:			JP 1993-46113	19930212

OTHER SOURCE(S): MARPAT 122:93024

AB The title compound consists of  $CmH_{2m+1}CHFCH_2O-1,4-C_6H_4CO_2-1,4-C_6H_4OCH_2CnF_{2n+1}$  (I; m, n = 1-20) or I (m = 6, n = 7). The compound is prepared by esterification of  $HO-1,4-C_6H_4OCH_2CnF_{2n+1}$  and  $CmH_{2m+1}CHFCH_2O-1,4-C_6H_4CO_2H$ . The liquid crystal composition contains smectic liquid crystal compds. and the claimed compound. The display is obtained by using the composition. The compound showed high spontaneous polarization and rapid response.

IT 160189-32-2

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(liquid crystal display containing perfluoroalkyloxyphenyl fluoroalkyloxybenzoate with high spontaneous polarization and rapid response)

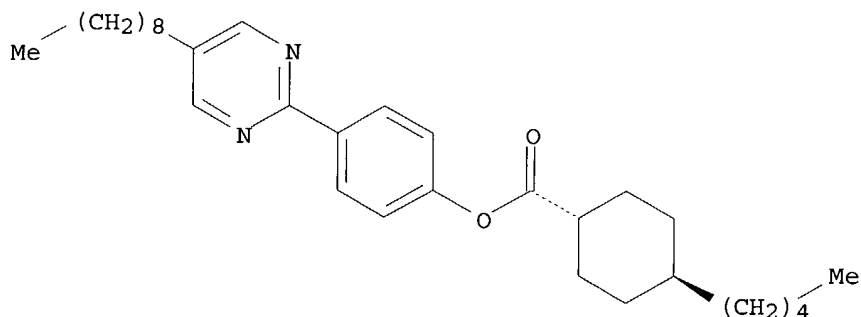
RN 160189-32-2 CAPLUS

CN Cyclohexanecarboxylic acid, 4-pentyl-, 4-(5-nonyl-2-pyrimidinyl)phenyl

09/ 811,359

ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



L11 ANSWER 53 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1995:207981 CAPLUS

DOCUMENT NUMBER: 122:93023

TITLE: Perfluoroalkoxyphenyl fluoroalkylbenzoate, its preparation, its-containing liquid crystal composition, and display

INVENTOR(S): Nohira, Hiroyuki; Sakaigawa, Akira; Imamura, Shinichi

PATENT ASSIGNEE(S): Idemitsu Petrochemical Co, Japan

SOURCE: Jpn. Kokai Tokyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06239800	A2	19940830	JP 1993-46114	19930212
PRIORITY APPLN. INFO.:			JP 1993-46114	19930212

OTHER SOURCE(S): MARPAT 122:93023

AB The title compound consists of  $C_mH_{2m+1}C(CF_3)H-1,4-C_6H_4CO_2-1,4-C_6H_4OCH_2C_nF_{2n+1}$  (I; m, n = 1-20) or I (m = 6, n = 7). The compound is prepared by esterification of  $HO-1,4-C_6H_4OCH_2C_nF_{2n+1}$  and  $C_mH_{2m+1}C(CF_3)H-1,4-C_6H_4CO_2H$ . The liquid crystal composition contains smectic liquid crystal compds. and the claimed compound. The display is obtained by using the composition. The compound showed high spontaneous polarization and rapid response.

IT 160189-32-2

RL: DEV (Device component use); TEM (Technical or engineered material use); USES (Uses)

(liquid crystal display containing perfluoroalkoxyphenyl fluoroalkylbenzoate with high spontaneous polarization and rapid response)

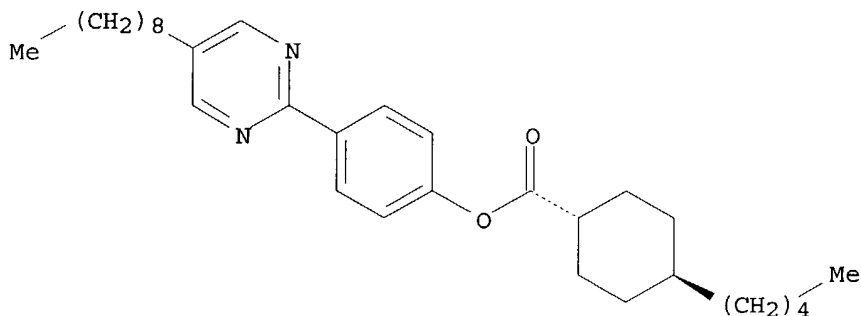
RN 160189-32-2 CAPLUS

CN Cyclohexanecarboxylic acid, 4-pentyl-, 4-(5-nonyl-2-pyrimidinyl)phenyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.



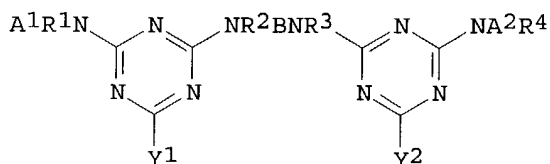
09/ 811,359



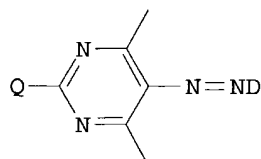
L11 ANSWER 54 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1994:485637 CAPLUS  
 DOCUMENT NUMBER: 121:85637  
 TITLE: Dyeing of cellulose-containing fiber materials with reactive dyes  
 INVENTOR(S): Landre, Jean Francois; Tzikas, Athanassios; Luttringer, Jean Pierre  
 PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.  
 SOURCE: PCT Int. Appl., 65 pp.  
 CODEN: PIXXD2  
 DOCUMENT TYPE: Patent  
 LANGUAGE: English  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9318224	A1	19930916	WO 1993-EP426	19930224
W: AU, BB, BG, BR, CA, CZ, FI, HU, JP, KP, KR, KZ, LK, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, UA, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, SN, TD, TG				
AU 9336297	A1	19931005	AU 1993-36297	19930224
AU 677575	B2	19970501		
EP 629249	A1	19941221	EP 1993-905272	19930224
EP 629249	B1	19970108		
R: BE, CH, DE, DK, ES, FR, GB, IT, LI, PT				
JP 07504949	T2	19950601	JP 1993-515289	19930224
ES 2098727	T3	19970501	ES 1993-905272	19930224
BR 9306026	A	19971118	BR 1993-6026	19930224
CA 2129750	C	20030506	CA 1993-2129750	19930224
US 5525124	A	19960611	US 1994-295765	19940902
PRIORITY APPLN. INFO.:			CH 1992-714	A 19920306
			CH 1992-715	A 19920306
			WO 1993-EP426	A 19930224

OTHER SOURCE(S): MARPAT 121:85637  
 GI



I



II

AB Title process comprises dyeing in a dyebath containing 0-20 g/L mineral acid salt, e.g., NaCl or Na<sub>2</sub>SO<sub>4</sub>, and  $\geq 1$  reactive dye (I) (A1 = dye chromophore, A2 = A1, H, colorless organic residue; R1-4 = H, unsubstituted C1-4 alkyl; B = aliphatic or aromatic bridging group; Y1, Y2 = F, carboxypyridinium) and (II) (Q = optionally substituted Ph, **naphthyl**, heteroaryl; D = diazo radical; R5, R6 = optionally substituted amino,  $\geq 1$  R5, R6, or D contains a fiber-reactive group). The process produces dyeings with good fastness and high color yields without the addition of large amts. of mineral acid salts.

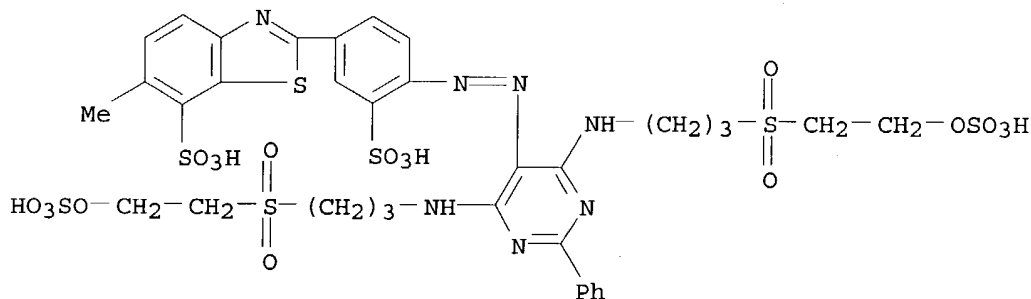
IT 156202-64-1

RL: USES (Uses)

(dyeing of cotton by, in presence of low amts. of mineral acid salts)

RN 156202-64-1 CAPLUS

CN 7-Benzothiazolesulfonic acid, 6-methyl-2-[4-[[2-phenyl-4,6-bis[[3-[[2-(sulfooxy)ethyl]sulfonyl]propyl]amino]-5-pyrimidinyl]azo]-3-sulphophenyl]]-(9CI) (CA INDEX NAME)



L11 ANSWER 55 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1994:408893 CAPLUS

DOCUMENT NUMBER: 121:8893

TITLE: **Phenyl**-substituted acrylate ester

agrochemical fungicides

INVENTOR(S): Mueller, Bernd; Roehl, Franz; Koenig, Hartmann; Sauter, Hubert; Lorenz, Gisela; Ammermann, Eberhard

PATENT ASSIGNEE(S): BASF A.-G., Germany

SOURCE: Eur. Pat. Appl., 86 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

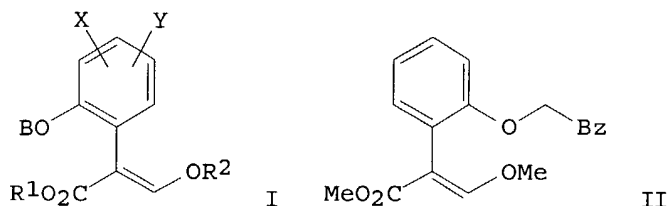
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 581095	A2	19940202	EP 1993-111103	19930712
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, NL, PT, SE				
CA 2100546	AA	19940125	CA 1993-2100546	19930714
JP 06211748	A2	19940802	JP 1993-181305	19930722
AU 9342121	A1	19940127	AU 1993-42121	19930723
AU 660226	B2	19950615		
HU 66105	A2	19940928	HU 1993-2150	19930723
ZA 9305332	A	19950123	ZA 1993-5332	19930723

PRIORITY APPLN. INFO.: DE 1992-4224457 19920724

OTHER SOURCE(S): MARPAT 121:8893

GI



AB The title compds. [I; B = (un)substituted alkyl, C1-4 (un)substituted alkenyl, (un)substituted alkynyl, etc.; R1, R2 = (un)substituted alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, etc.; X, Y = H, halogen, CN, NO2, haloalkyl, alkyl, alkenyl, alkynyl, heteroaryl, heterocyclyl, etc.], useful as agrochem. fungicides, are prepared and I-containing formulations presented. Thus, Me  $\alpha$ -(2-hydroxyphenyl)- $\beta$ -methoxyacrylate was condensed with phenacyl bromide, producing acrylate II, m.p. 76°, which demonstrated 90% inhibitory activity against *Plasmopara viticola* at 250 ppm.

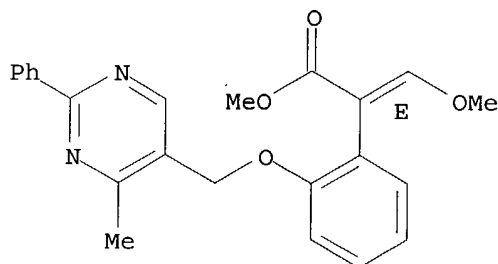
IT 154594-91-9P

RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES (Uses) (preparation of, as agrochem. fungicide)

RN 154594-91-9 CAPLUS

CN Benzeneacetic acid,  $\alpha$ -(methoxymethylene)-2-[(4-methyl-2-phenyl-5-pyrimidinyl)methoxy]-, methyl ester, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L11 ANSWER 56 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:614448 CAPLUS

DOCUMENT NUMBER: 119:214448

TITLE: Preparation of optically active aromatic esters and liquid crystal compositions containing them

INVENTOR(S): Azumai, Takayuki; Toda, Shoji; Minamii, Masayoshi

PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokyo Koho, 6 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

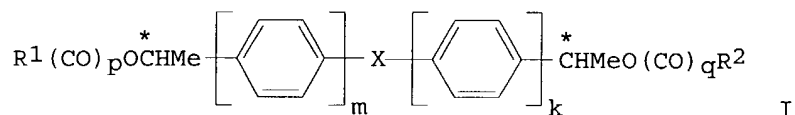
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04337384	A2	19921125	JP 1991-110116	19910515
JP 2906729	B2	19990621		
PRIORITY APPLN. INFO.:			JP 1991-110116	19910515

09/ 811,359

OTHER SOURCE(S): MARPAT 119:214448  
GI



AB The title compds. I (X = CO<sub>2</sub>, O<sub>2</sub>C; R<sub>1</sub>, R<sub>2</sub> = halo, C<sub>1</sub>-20 alkyl, C<sub>2</sub>-20 alkoxy; m, k, l = 1, 2; p, q = 0, 1; C\* denotes an asym. C atom) are prepared. Liquid crystal compns. contain I for use in liquid-crystal display devices. When I are mixed to form chiral smectic C liquid crystal compns., I induce sufficient spontaneous polarization, improve orientation, and provide ferroelec. liquid crystal materials. A total of 6 optically active Ph benzoates were prepared.

IT 150742-81-7

RL: PRP (Properties)

(liquid crystal composition, for display)

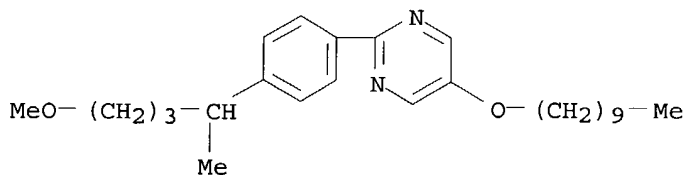
RN 150742-81-7 CAPLUS

CN Pyrimidine, 5-(decyloxy)-2-[4-(4-methoxy-1-methylbutyl)phenyl]-, mixt. with 5-(decyloxy)-2-[4-(5-methoxypentyl)phenyl]pyrimidine (9CI) (CA INDEX NAME)

CM 1

CRN 150742-80-6

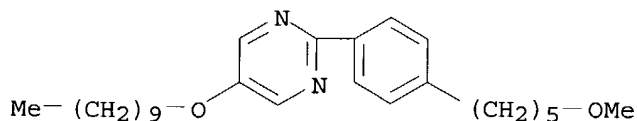
CMF C26 H40 N2 O2



CM 2

CRN 150742-79-3

CMF C26 H40 N2 O2



L11 ANSWER 57 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:614343 CAPLUS

DOCUMENT NUMBER: 119:214343

TITLE: Synthesis and properties of optically active 1,3-diols and their derivatives as chiral dopants for ferroelectric liquid crystals

AUTHOR(S): Kusumoto, Tetsuo; Sato, Kenichi; Ogino, Kumiko; Hiyama, Tamejiro; Takehara, Sadao; Osawa, Masashi;

09/ 811,359

CORPORATE SOURCE: Nakamura, Kayoko  
Sagami Chem. Res. Cent., Sagamihara, 229, Japan  
SOURCE: Liquid Crystals (1993), 14(3), 727-32  
CODEN: LICRE6; ISSN: 0267-8292

DOCUMENT TYPE: Journal  
LANGUAGE: English

AB New chiral dopants  $\beta$ -hydroxy ketones (I), 1,3-diols (II), 1,3-dioxanes (III) and 1,3-dioxan-2-ones (IV) were designed and synthesized. Reaction of (R)-1,2-epoxyoctane with carbanions derived from 2-(4-substituted **phenyl**)-1,3-dithianes followed by hydrolysis of the resulting hydroxy dithianes afforded I. Reduction of I gave the diols II, which yielded III upon acetalization and IV upon carbonation. The syn isomers of II, III, and IV exhibited larger spontaneous polarizations, when applied as chiral dopants, than the anti isomers or hydroxy ketones I.

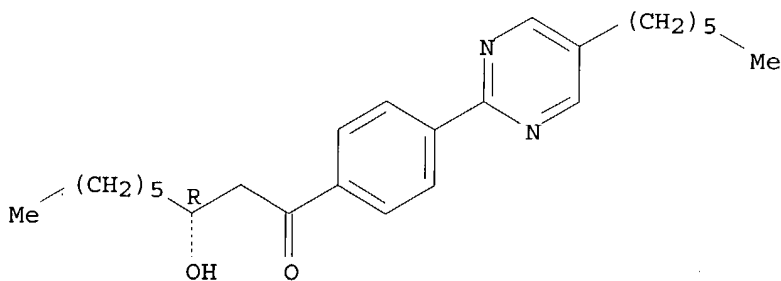
IT 145747-60-0

RL: PRP (Properties)  
(as chiral dopant for ferroelec. liquid crystals, synthesis and properties of)

RN 145747-60-0 CAPLUS

CN 1-Nonanone, 1-[4-(5-hexyl-2-pyrimidinyl)phenyl]-3-hydroxy-, (R)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 58 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:254557 CAPLUS

DOCUMENT NUMBER: 118:254557

TITLE: Preparation of 2-**phenyl**-4-fluoroalkanenitrile derivatives, liquid crystal compositions containing them, and liquid crystal display devices

INVENTOR(S): Takehara, Sadao; Osawa, Masashi; Nakamura, Kayoko; Hiyama, Tamejiro; Kusumoto, Tetsuo; Nakayama, Akiko; Nishide, Kyoji

PATENT ASSIGNEE(S): Dainippon Ink and Chemicals, Inc., Japan; Sagami Chemical Research Center

SOURCE: Jpn. Kokai Tokyo Koho, 9 pp.  
CODEN: JKXXAF

DOCUMENT TYPE: Patent

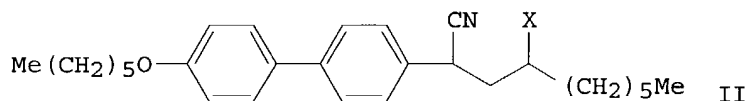
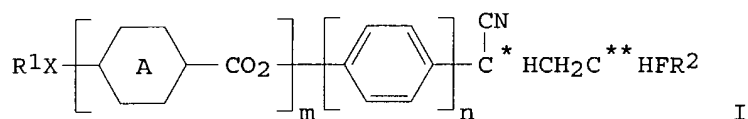
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04327567	A2	19921117	JP 1991-125448	19910426
PRIORITY APPLN. INFO.:			JP 1991-125448	19910426
OTHER SOURCE(S):		MARPAT 118:254557		

GI



AB The title compds. [I; R1, R2 = C1-18 alkyl; X = O, CO2, single bond; ring A = (un)substituted 1,4-phenylene, trans-cyclohexylene; C\*, C\*\* = asym. C atoms independently having (R) or (S) configuration; m = 0, 1; n = 1, 2] are prepared. When a small amount of I is added as a chiral dopant to a mother liquid crystal having smectic C phase, it induces a large spontaneous polarization and provides a ferroelec. chiral smectic liquid crystal composition with high response speed over a broad temperature range, good orientation property, and chemical stability towards H2O and light, which make it useful as a material for optical switching display devices. Thus, lithiation of 4-(4-n-hexyloxyphenyl)phenylacetonitrile with BuLi in HMPA-hexane-THF at -78° followed by addition to 1,2-epoxyoctane with warming to room temperature over 3 h gave biphenylhydroxydecanenitrile derivative 45% (2S,4R)-II (X = OH) of 93% e.e. and 30% (2R,4R)-isomer of 93% e.e. which were fluorinated with Et2NSF3 in CH2Cl2 at -78° to 0° for 3 h to give 86% (2S,4S)-II (X = F) of 97% e.e. and 66% (2R,4R)-II (X = F) (III) of 98% e.e., resp. A liquid crystal composition containing 10% III and 90% of a mixture of 4-phenylpyrimidine derivs. showed chiral smectic C to smectic A transition at 58°, tilt angle 18.8°, spontaneous polarization +7.0 nC/cm2, and electrooptical response speed 88 μs.

IT 147553-34-2

RL: RCT (Reactant); RACT (Reactant or reagent)  
(ferroelec. liquid crystal composition, for display)

RN 147553-34-2 CAPLUS

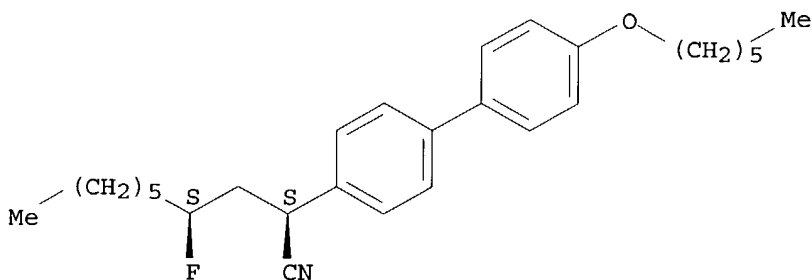
CN [1,1'-Biphenyl]-4-acetonitrile, α-(2-fluorooctyl)-4'-(hexyloxy)-, [S-(R\*,R\*)]-, mixt. with 2-[4-(decyloxy)phenyl]-5-octylpyrimidine, 2-[2-fluoro-4-(octyloxy)phenyl]-5-(4-heptylphenyl)pyrimidine, 2-[4-(nonyloxy)phenyl]-5-octylpyrimidine and 5-octyl-2-[4-(octyloxy)phenyl]pyrimidine (9CI) (CA INDEX NAME)

CM 1

CRN 147224-04-2

CMF C28 H38 F N O

Absolute stereochemistry.

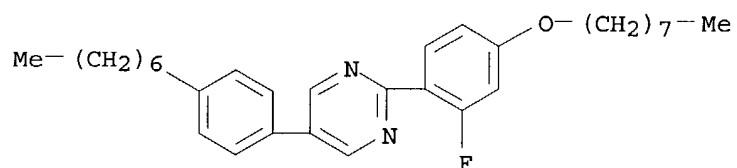


09/ 811,359

CM 2

CRN 124257-09-6

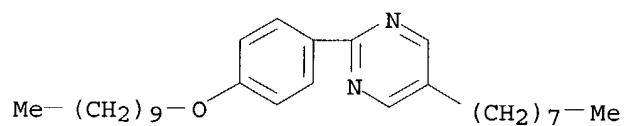
CMF C31 H41 F N2 O



CM 3

CRN 57202-52-5

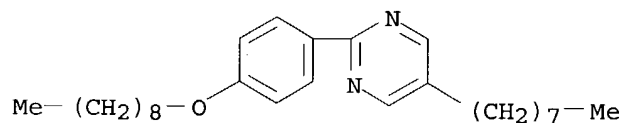
CMF C28 H44 N2 O



CM 4

CRN 57202-51-4

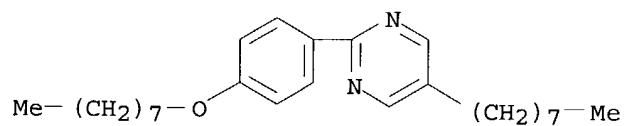
CMF C27 H42 N2 O



CM 5

CRN 57202-50-3

CMF C26 H40 N2 O



L11 ANSWER 59 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1993:14113 CAPLUS

DOCUMENT NUMBER: 118:14113

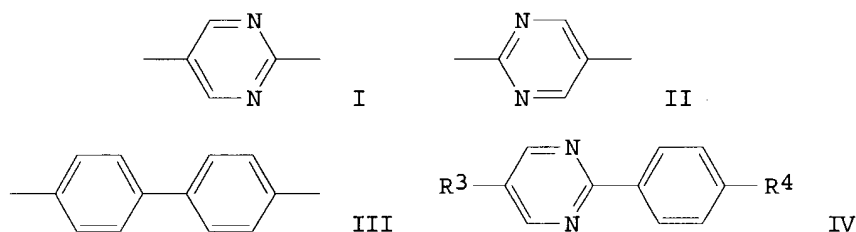
TITLE: Ferroelectric liquid crystal composition

INVENTOR(S): Saito, Goro; Yoshio, Kunikyo; Sato, Masahiro;  
Watanabe, Tetsuya

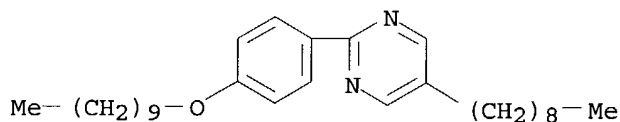
09/ 811,359

PATENT ASSIGNEE(S): NEC Corp., Japan; Sanyo Chemical Industries Ltd.  
SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04126793	A2	19920427	JP 1990-249176	19900919
PRIORITY APPLN. INFO.: GI			JP 1990-249176	19900919



AB The title liquid-crystal composition comprises  $\geq 1$  R1(XA)nYD(CH2)mC(CN)HR2  
[R1,2 = C1-20 alkyl; X = O, single bond; Y = single bond, O, CO2, OCO,  
CH2O, OCH2, C.tplbond.C, CH2CH2; A = p-C6H4, I, II, III, 2,6-  
**naphthyl**; D = 2,6-**naphthyl**; n = 0,1] and  $\geq 1$  IV  
[R3,4 = C1-15 alkyl or alkoxy].  
IT **144806-56-4**  
RL: USES (Uses)  
(ferroelec. liquid-crystal composition containing)  
RN 144806-56-4 CAPLUS  
CN Pyrimidine, 2-[4-(decyloxy)phenyl]-5-nonyl- (9CI) (CA INDEX NAME)

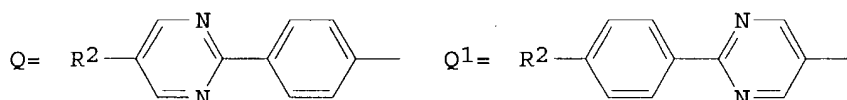


L11 ANSWER 60 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1992:612517 CAPLUS  
DOCUMENT NUMBER: 117:212517  
TITLE: Preparation of optically active 2-phenylpyrimidine  
derivatives, liquid crystal compositions containing  
them, and liquid crystal electrooptical devices  
INVENTOR(S): Mihashi, Shigeru; Matsushima, Yoshimasa; Imai,  
Takashi; Mori, Kiichi; Yamada, Mamoru; Sugiyama,  
Hiroshi; Yagi, Misao; Kondo, Hitoshi; Hagiwara,  
Toshimitsu  
PATENT ASSIGNEE(S): Takasago Perfumery Co., Ltd., Japan  
SOURCE: Jpn. Kokai Tokkyo Koho, 58 pp.  
CODEN: JKXXAF  
DOCUMENT TYPE: Patent  
LANGUAGE: Japanese  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:



09/ 811,359

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04154769	A2	19920527	JP 1990-279079	19901019
JP 2627679	B2	19970709		
US 6093345	A	20000725	US 1993-91406	19930714
PRIORITY APPLN. INFO.:			JP 1990-279079	A 19901019
			US 1991-779528	B1 19911018
OTHER SOURCE(S):			MARPAT 117:212517	
GI				



AB Optically active AO(CH<sub>2</sub>)<sub>n</sub>C\*HF(CH<sub>2</sub>)<sub>m</sub>C\*HXR1 (I; C\* = asym. C atom; R1 = linear C2-5 alkyl; n = 1, 2; m = 0-3; X = F, Me; A = Q, Q1; R2 = linear C8-12 alkyl), useful as chiral dopants for nematic liquid crystals, are prepared. A liquid crystal composition contains at least one I and a liquid crystal electrooptical device is obtained by injecting the latter composition. Thus, 2-(4-hydroxyphenyl)-5-decylpyrimidine 3.0, (2R,5S)-2-tetrahydropyranyloxy-5-methylheptyl p-toluenesulfonate (preparation given) 6.0, K<sub>2</sub>CO<sub>3</sub> 2.1 g and 75 mL DMF were stirred for 18 h to give 77.5% (2'R,5'S)-2-[4-(2'-tetrahydropyranyloxy-5-methylheptyloxy)phenyl]-5-decylpyrimidine which was deprotected by p-toluenesulfonic acid in MeOH to give 68.2% an alc. and then fluorinated by hexafluoropropene-Et<sub>2</sub>NH adduct in CH<sub>2</sub>Cl<sub>2</sub> to give 46.5% (2'S,5'S)-2-[4-(2'-fluoro-5'-methylheptyloxy)phenyl]-5-decylpyrimidine (II). II showed SC\*-SA phase transition temperature 42.0° and a liquid crystal composition containing 9.3 mol% showed spontaneous polarization 3.1 nC/cm<sup>2</sup>, tilt angle 14°, and response speed 46 μs at TC-5°.

IT 144115-31-1

RL: RCT (Reactant); RACT (Reactant or reagent)  
(liquid crystal composition, for display device)

RN 144115-31-1 CAPLUS

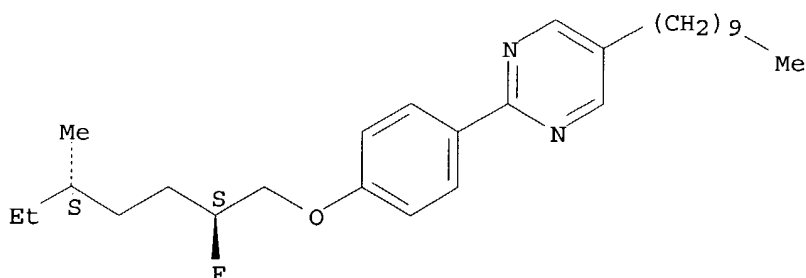
CN Pyrimidine, 5-decyl-2-[4-[(2-fluoro-5-methylheptyl)oxy]phenyl]-, [S-(R\*,R\*)]-, mixt. with 2-[4-(decyloxy)phenyl]-5-octylpyrimidine, 5-heptyl-2-[4-(nonyloxy)phenyl]pyrimidine, 5-hexyl-2-[4-(octyloxy)phenyl]pyrimidine, 2-[4-(hexyloxy)phenyl]-5-octylpyrimidine and 5-octyl-2-[4-(octyloxy)phenyl]pyrimidine (9CI) (CA INDEX NAME)

CM 1

CRN 144088-30-2

CMF C28 H43 F N2 O

Absolute stereochemistry.

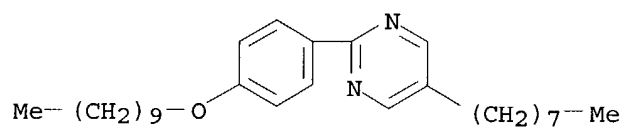


09/ 811,359

CM 2

CRN 57202-52-5

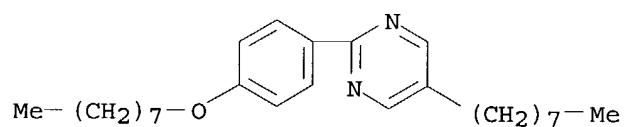
CMF C28 H44 N2 O



CM 3

CRN 57202-50-3

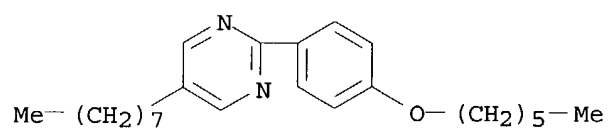
CMF C26 H40 N2 O



CM 4

CRN 57202-48-9

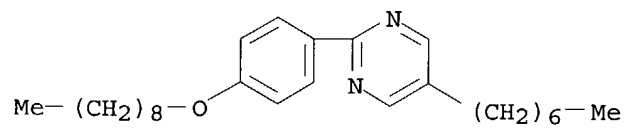
CMF C24 H36 N2 O



CM 5

CRN 57202-40-1

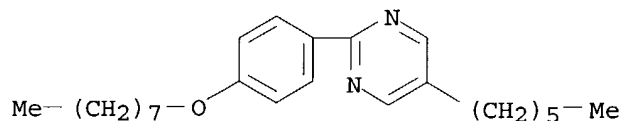
CMF C26 H40 N2 O



CM 6

CRN 57202-30-9

CMF C24 H36 N2 O



L11 ANSWER 61 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1992:83522 CAPLUS

DOCUMENT NUMBER: 116:83522

TITLE: Optically active **phenyl**(hydroxymethyl)-  
 $\gamma$ -butyrolactones and liquid crystal compositions  
 containing them

INVENTOR(S): Sakashita, Keiichi; Hayashi, Shoji; Kamimura, Shigeo;  
 Mori, Kenji

PATENT ASSIGNEE(S): Mitsubishi Rayon Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 15 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

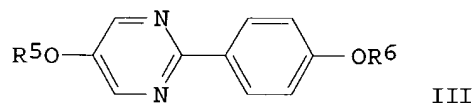
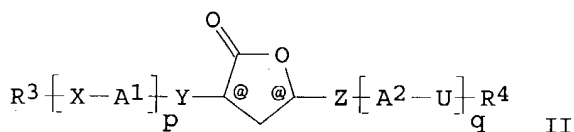
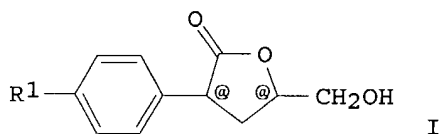
LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03173879	A2	19910729	JP 1990-189223	19900717
PRIORITY APPLN. INFO.:			JP 1989-185769	19890718
OTHER SOURCE(S):		MARPAT 116:83522		

GI



AB The title compds. [I; II; R1 = OH, CO<sub>2</sub>H, HOCH<sub>2</sub>, alkyl, alkoxy; R3, R4 = alkyl, alkenyl, alkynyl, alkoxyalkyl, alkylthioalkyl, etc.; X, U = O, CO<sub>2</sub>, O<sub>2</sub>C; Y, Z = single bond, O, CO<sub>2</sub>, O<sub>2</sub>C, CH<sub>2</sub>O, OCH<sub>2</sub>, A1, A2 = (substituted) phenylene, heteracyclohexylene, etc.; p, q = 0, 1; asterisk indicates chiral center] are prepared for liquid crystal compns. A solution of (S,S)-2-hydroxy-4-(butoxymethyl)- $\gamma$ -butyrolactone, 4-[4-(undecanoyloxy)phenoxymethyl]benzoic acid, PPh<sub>3</sub>, and di-Et azodicarboxylate in benzene was allowed to react at room temperature overnight to give the corresponding title ester. A liquid crystal composition containing this and phenylpyrimidines III [R5 = C<sub>8</sub>H<sub>17</sub>, R6 = C<sub>6</sub>H<sub>13</sub>, C<sub>8</sub>H<sub>17</sub>, C<sub>12</sub>H<sub>25</sub>, C<sub>11</sub>H<sub>23</sub>; R5 = C<sub>6</sub>H<sub>13</sub>, R6 = C<sub>10</sub>H<sub>21</sub>, C<sub>9</sub>H<sub>19</sub>, C<sub>8</sub>H<sub>17</sub>] had transition temps. of -10, 62,

09/ 811,359

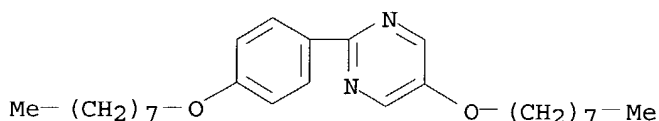
72 and 77° between crystalline and chiral smectic C phases, chiral smectic C and smectic A phases, smectic A and Ch phases, and Ch and Iso phases whereas a composition containing only III had transition temps. of 1, 63, 78, and 81°, resp.

IT 114767-84-9

RL: RCT (Reactant); RACT (Reactant or reagent)  
(liquid crystal comps. containing)

RN 114767-84-9 CAPLUS

CN Pyrimidine, 5-(octyloxy)-2-[4-(octyloxy)phenyl]- (9CI) (CA INDEX NAME)



L11 ANSWER 62 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1991:667057 CAPLUS

DOCUMENT NUMBER: 115:267057

TITLE: Preparation of optically active  
(aryl)trifluoromethylalkyl alkanoates and ethers for  
liquid-crystal compositions

INVENTOR(S): Kurimoto, Isao; Higashii, Takayuki; Toda, Shoji;  
Minai, Masayoshi; Sekine, Chizu; Tani, Takeshi;  
Fujisawa, Koichi

PATENT ASSIGNEE(S): Sumitomo Chemical Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 90 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

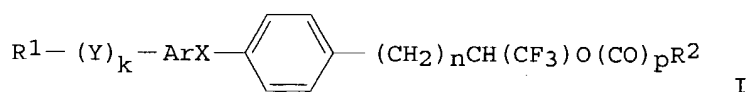
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 434297	A2	19910626	EP 1990-313537	19901212
EP 434297	A3	19911106		
EP 434297	B1	19961016		
R: CH, DE, FR, GB, LI				
JP 03294246	A2	19911225	JP 1990-231539	19900829
JP 2864698	B2	19990303		
US 5238598	A	19930824	US 1990-626980	19901213
PRIORITY APPLN. INFO.:			JP 1989-329085	19891218
			JP 1990-231539	19900829
			JP 1989-234381	19890908

OTHER SOURCE(S): MARPAT 115:267057

GI



AB Optically active title compds. I [R<sub>1</sub> = C<sub>3</sub>-26 alkyl; R<sub>2</sub> = (halo) C<sub>1</sub>-20 alkyl or alkoxyalkyl; Ar = 1,4-phenylene, 4,4'-biphenylene, etc.; X = COO when n = 0 and COO or OCO when n = 1-5; Y = O, COO, OCO; k = 0,1; n = 0-5; p = 0, 1], useful for liquid crystal comps., were prepared Thus, 4-benzyloxy- $\alpha,\alpha,\alpha$ -trifluoroacetylphenone (preparation given)

was subjected to NaBH<sub>4</sub> reduction, acetylation of the alc. formed, and asym. hydrolysis to give (+)-4-benzyloxy-1-(1-acetoxy-2,2,2-trifluoroethyl)benzene. Alkylation by n-hexyl tosylate followed by debenzoylation gave (+)-4-(1-hexyloxy-2,2,2-trifluoroethyl)phenol. This was stirred at room temperature for 24 h with 4-decyloxybenzene acid, DCC and anhydrous CH<sub>2</sub>Cl<sub>2</sub> to give (+)-4-(1-hexyloxy-2,2,2-trifluoroethyl)phenyl 4-decyloxybenzoate (II). A liquid-crystal composition containing 20% II gave spontaneous polarization of -13 nC/cm<sup>2</sup> at 20°.

IT 137614-98-3P

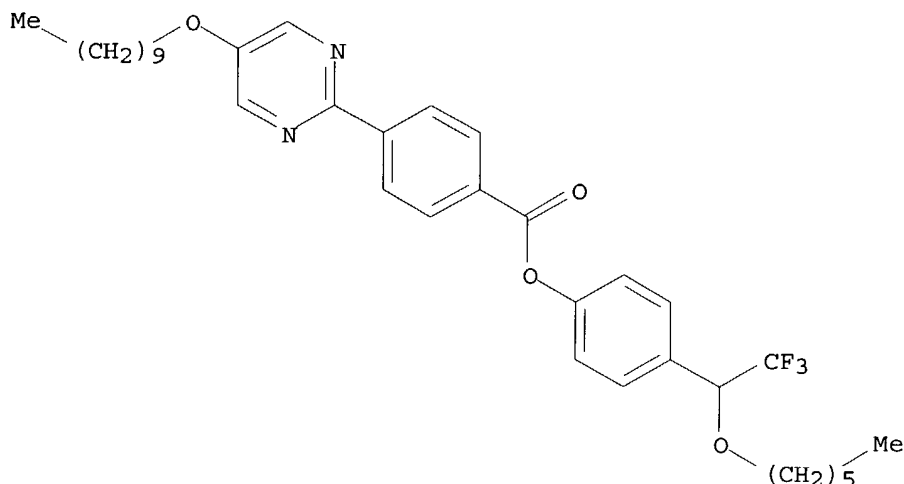
RL: PREP (Preparation)

(preparation of, for liquid-crystal electrooptical display devices)

RN 137614-98-3 CAPLUS

CN Benzoic acid, 4-[5-(decyloxy)-2-pyrimidinyl]-, 4-[2,2,2-trifluoro-1-(hexyloxy)ethyl]phenyl ester, (+)-(9CI) (CA INDEX NAME)

Rotation (+).



L11 ANSWER 63 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:581603 CAPLUS

DOCUMENT NUMBER: 113:181603

TITLE: Optically-active 2-[4-(6-chloro-4-methylalkoxy)phenyl]-5-alkoxypyrimidines as chiral smectic liquid crystals

INVENTOR(S): Shibata, Toshihiro; Kimura, Masaki

PATENT ASSIGNEE(S): Adeka Argus Chemical Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 3 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 02117667	A2	19900502	JP 1988-271752	19881027
PRIORITY APPLN. INFO.:			JP 1988-271752	19881027

GI For diagram(s), see printed CA Issue.

AB The title compds. I (R = C1-18 n-alkyl; R1 = H, C1-11 alkyl) are claimed. I show a chiral smectic phase at lower mesomorphic range than similar phenylpyrimidine derivs. in which 6-chloro-4-methylalkoxy are substituted with 4-methylhexyloxy, thus ferroelec. liquid-crystal compns. containing I are useful for electrooptical devices, such as liquid-crystal display. (+)-EtCHClCH<sub>2</sub>CHMe(CH<sub>2</sub>)<sub>3</sub>OH was treated with 2-(4-hydroxyphenyl)-5-

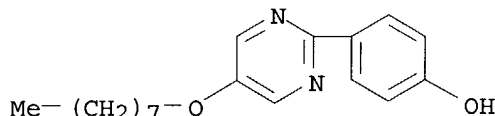
09/ 811,359

octyloxypyrimidine to give I (R = octyl, R1 = Et) (II), showing a chiral smectic C phase. A liquid-crystal display cell packed with II was prepared

IT 104539-91-5, 2-(4-Hydroxyphenyl)-5-octyloxypyrimidine  
RL: RCT (Reactant); RACT (Reactant or reagent)  
(etherification of, with optically-active chloromethyloctanol, chiral smectic C liquid crystal from)

RN 104539-91-5 CAPLUS

CN Phenol, 4-[5-(octyloxy)-2-pyrimidinyl]- (9CI) (CA INDEX NAME)



L11 ANSWER 64 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:524525 CAPLUS

DOCUMENT NUMBER: 113:124525

TITLE: Optically active esters of 5-ethyl- and 5-vinyl-1,3-dioxolan-4-carboxylic acid, their preparation, their use as dopants in liquid-crystal mixtures, and liquid-crystal mixtures and display devices containing them

INVENTOR(S): Mueller, Ingrid; Duebal, Hans Rolf; Escher, Klaus; Hemmerling, Wolfgang; Illian, Gerhard; Murakami, Mikio; Ohlendorf, Dieter; Wingen, Rainer

PATENT ASSIGNEE(S): Hoechst A.-G., Germany

SOURCE: Ger. Offen., 13 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3832503	A1	19900329	DE 1988-3832503	19880924
EP 361272	A1	19900404	EP 1989-117265	19890919
EP 361272	B1	19940601		
R: AT, BE, CH, DE, FR, GB, IT, LI, NL, SE				
AT 106402	E	19940615	AT 1989-117265	19890919
NO 8903778	A	19900326	NO 1989-3778	19890922
JP 02129179	A2	19900517	JP 1989-245378	19890922
US 5328638	A	19940712	US 1992-881520	19920512
PRIORITY APPLN. INFO.:			DE 1988-3832503	19880924
			EP 1989-117265	19890919
			US 1989-410949	19890922

OTHER SOURCE(S): CASREACT 113:124525; MARPAT 113:124525

AB Tilted smectic liquid-crystal phases containing compds. of the invention as dopants had spontaneous polarization 50-100% higher than when they were doped with known compds. (4R,5R)-4-(5-n-Octylpyrimidin-2-yl)phenyl 2,2-dimethyl-5-vinyl-1,3-dioxolan-4-carboxylate was prepared from 4-(5-n-octylpyrimidin-2-yl)phenol and 2,2-dimethyl-5-vinyl-1,3-dioxolan-4-carboxylic acid.

IT 129293-92-1P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, as dopant for liquid-crystal mixture)

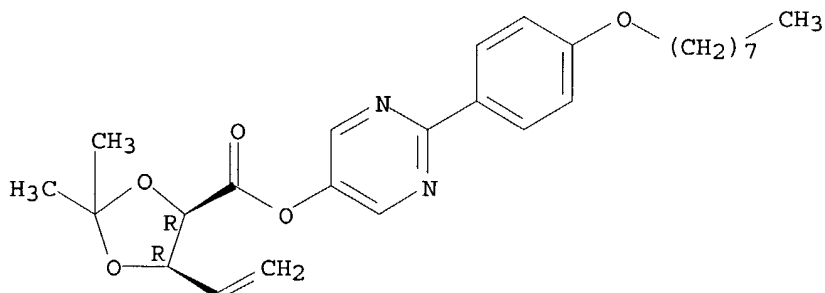
RN 129293-92-1 CAPLUS

CN 1,3-Dioxolane-4-carboxylic acid, 5-ethenyl-2,2-dimethyl-, 2-[4-(octyloxy)phenyl]-5-pyrimidinyl ester, (4R-cis)- (9CI) (CA INDEX

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NAME)

Absolute stereochemistry.



L11 ANSWER 65 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:227426 CAPLUS

DOCUMENT NUMBER: 112:227426

TITLE:  $\alpha$ -(4-Substituted- **phenyl**)ethyl alcohol  
derivatives and liquid-crystal compositions containing  
them

INVENTOR(S): Kodon, Mitsuhiro; Kuratate, Tomoaki; Funada, Fumiaki

PATENT ASSIGNEE(S): Sharp Corp., Japan

SOURCE: Ger. Offen., 15 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

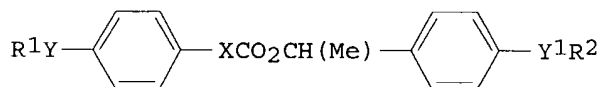
LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3907507	A1	19890921	DE 1989-3907507	19890308
DE 3907507	C2	19900823		
JP 02019345	A2	19900123	JP 1988-169951	19880706
JP 02036152	A2	19900206	JP 1988-183924	19880722
JP 02040342	A2	19900209	JP 1988-191165	19880729
JP 01316348	A2	19891221	JP 1988-332349	19881229
JP 05088698	B4	19931224		
GB 2216371	A1	19891011	GB 1989-5403	19890309
GB 2216371	B2	19920708		
US 5209867	A	19930511	US 1991-815580	19911230
PRIORITY APPLN. INFO.:			JP 1988-57295	19880310
			JP 1988-169951	19880706
			JP 1988-183924	19880722
			JP 1988-191165	19880729
			US 1989-321079	19890309
			US 1991-701346	19910505

GI



I

AB The title derivs. have the general formula I, where R1, R2 = C1-12 linear or branched alkyl; X = a single bond, 1,4-phenylene, or CH2; and Y, Y1 = a single bond or O.

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IT 126130-05-0P

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of, for smectic C liquid-crystal mixts.)

RN 126130-05-0 CAPLUS

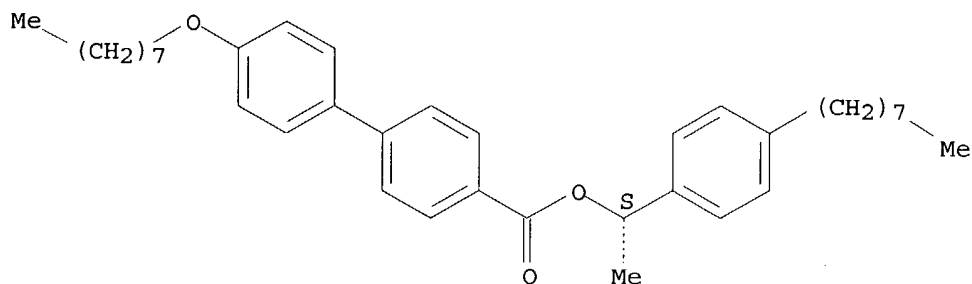
CN [1,1'-Biphenyl]-4-carboxylic acid, 4'-hexyl-, 4-(hexyloxy)phenyl ester, mixt. with 2-(4-butoxyphenyl)-5-hexylpyrimidine, 4-(hexyloxy)phenyl 4-(octyloxy)benzoate, 2-[4-(2-methylbutoxy)phenyl]-5-(undecyloxy)pyrimidine, 2-[4-[(4-methylhexyl)oxy]phenyl]-5-octylpyrimidine, 2-[4-[(6-methyloctyl)oxy]phenyl]-5-octylpyrimidine, 2-[4-[(3-methylpentyl)oxy]phenyl]-5-octylpyrimidine, 2-[4-[(3-methylpentyl)oxy]phenyl]-5-(undecyloxy)pyrimidine and 1-(4-octylphenyl)ethyl 4'-(octyloxy)[1,1'-biphenyl]-4-carboxylate (9CI) (CA INDEX NAME)

CM 1

CRN 126050-34-8

CMF C37 H50 O3

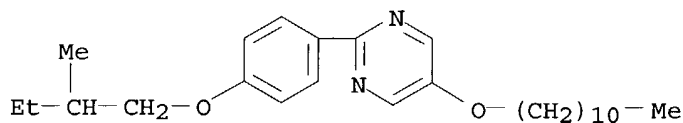
Absolute stereochemistry.



CM 2

CRN 118994-47-1

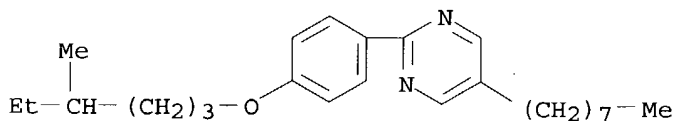
CMF C26 H40 N2 O2



CM 3

CRN 116020-57-6

CMF C25 H38 N2 O

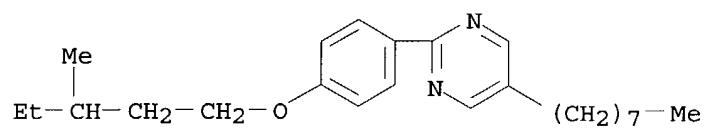


CM 4



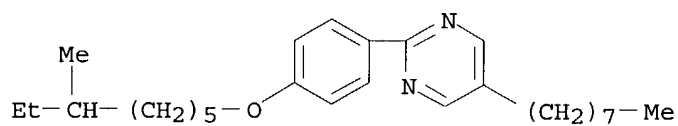
09/ 811,359

CRN 116020-50-9  
CMF C24 H36 N2 O



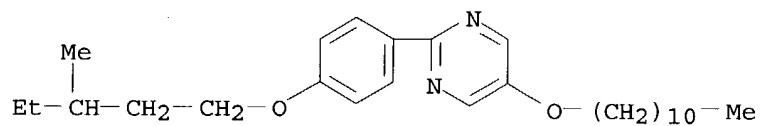
CM 5

CRN 108572-57-2  
CMF C27 H42 N2 O



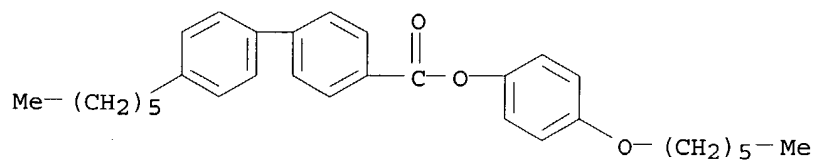
CM 6

CRN 108572-55-0  
CMF C27 H42 N2 O2



CM 7

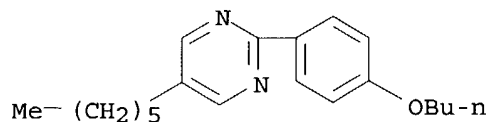
CRN 62268-66-0  
CMF C31 H38 O3



CM 8

CRN 57202-27-4  
CMF C20 H28 N2 O

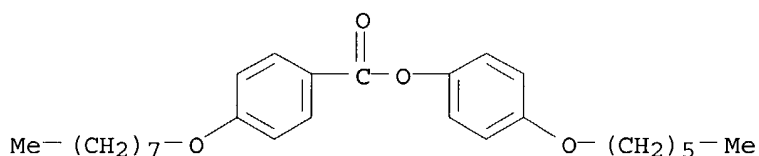
09/ 811,359



CM 9

CRN 54963-63-2

CMF C27 H38 O4



L11 ANSWER 66 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1990:210534 CAPLUS

DOCUMENT NUMBER: 112:210534

TITLE: Chemiluminescent determination of antiradical activity of chemicals. II. 5-Hydroxypyrimidines

AUTHOR(S): Zolotov, N. N.; Zalilov, K. Yu.; Mukhtarov, V. E.; Gashev, S. B.; Smirnov, L. D.; Dyumaev, K. M.

CORPORATE SOURCE: NII Farmakol., Moscow, USSR

SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1990), 24(1), 15-17

CODEN: KHFZAN; ISSN: 0023-1134

DOCUMENT TYPE: Journal

LANGUAGE: Russian

AB The antiradical activity of several alkyl and aryl derivs. of 5-hydroxypyrimidine was measured in a chemiluminescence system containing 3-hydroxypyridine, H<sub>2</sub>O<sub>2</sub>, and horseradish peroxidase. The results were compared with the data on luminescence quenching and lipophilicity of the agents determined by liquid chromatog. The structure-activity relationships are discussed. The results also correlated with reported data on cyclic nucleotide phosphodiesterase inhibition by the derivs. An immunostimulating activity of the compds. is suggested.

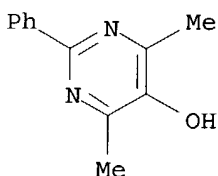
IT 75078-30-7, 2-Phenyl-4,6-dimethyl-5-hydroxypyrimidine

RL: PRP (Properties)

(antioxidant effects of, lipophilicity and structure in relation to)

RN 75078-30-7 CAPLUS

CN 5-Pyrimidinol, 4,6-dimethyl-2-phenyl- (6CI, 9CI) (CA INDEX NAME)



L11 ANSWER 67 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1989:85747 CAPLUS

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DOCUMENT NUMBER: 110:85747  
TITLE: Use of optically active 1,3-dioxolan-4 carboxylic acid esters as dopants in liquid-crystal mixtures new optically active esters, and liquid-crystal mixtures and electrooptical devices containing them  
INVENTOR(S): Wingen, Rainer; Duebal, Hans Rolf; Escher, Claus; Hemmerling, Wolfgang; Mueller, Ingrid; Ohlendorf, Dieter  
PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.  
SOURCE: Ger. Offen., 9 pp.  
CODEN: GWXXBX  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 1  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 3713273	A1	19881103	DE 1987-3713273	19870418
EP 288813	A1	19881102	EP 1988-105777	19880412
EP 288813	B1	19901114		
R: AT, BE, CH, DE, ES, FR, GB, IT, LI, NL, SE				
AT 58394	E	19901115	AT 1988-105777	19880412
NO 8801659	A	19881019	NO 1988-1659	19880415
NO 170885	B	19920914		
NO 170885	C	19921223		
CA 1339994	A1	19980811	CA 1988-564256	19880415
JP 63304088	A2	19881212	JP 1988-92682	19880416
JP 07017908	B4	19950301		
US 5641428	A	19970624	US 1992-879147	19920430
PRIORITY APPLN. INFO.:			DE 1987-3713273	19870418
			EP 1988-105777	19880412
			US 1988-181925	19880415
			US 1990-494909	19900309

OTHER SOURCE(S): CASREACT 110:85747

AB The optically active 1,3-dioxolan-4-carboxylic acid esters lead to ferroelec. liquid-crystal phases with short switching times and to electroclinic phases with large electroclinic coeffs. Their special advantage is that they induce a helix with a very large pitch, so that helix compensation by further dopants is unnecessary. These esters also have high UV stability. 4-(2-n-Octylpyrimidine-5-yl)phenol was reacted with 2,2-dimethyl-1,3-dioxolan-4-carboxylic acid chloride to form (R)-4-(2-n-octylpyrimidine-5-yl)**phenyl** 2,2-dimethyl-1,3-dioxolan-4-carboxylate, m. 88° and having optical rotation  $[\alpha]_{D3} = +7.54$ .

IT 118808-39-2P

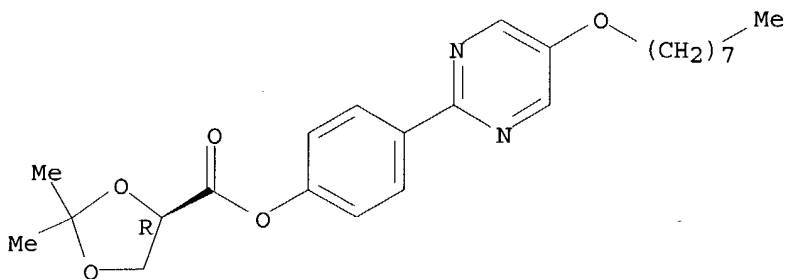
RL: PREP (Preparation)

(preparation of, for liquid-crystal phases for electrooptical devices)

RN 118808-39-2 CAPLUS

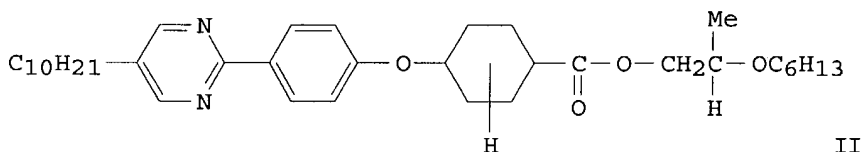
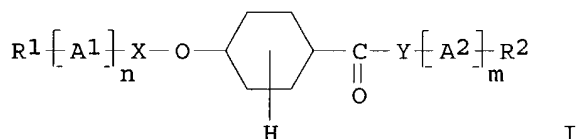
CN 1,3-Dioxolane-4-carboxylic acid, 2,2-dimethyl-, 4-[5-(octyloxy)-2-pyrimidinyl]phenyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L11 ANSWER 68 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN  
 ACCESSION NUMBER: 1989:15974 CAPLUS  
 DOCUMENT NUMBER: 110:15974  
 TITLE: Ferroelectric liquid-crystal display device  
 INVENTOR(S): Yamashita, Masataka; Yamada, Yoko; Kadokano, Goji;  
 Hioki, Cheko; Iwaki, Takashi  
 PATENT ASSIGNEE(S): Canon K. K., Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 63137986	A2	19880609	JP 1986-283476	19861128
PRIORITY APPLN. INFO.: GI			JP 1986-283476	19861128



AB The title device uses I (R1, R2 = chain radical; A1, A2 = divalent radical containing six-membered ring(s); X, Y = bond or divalent chain radical; n, m = 0 .apprx. 1 with n + m = 1) in the liquid crystal layer. Thus, a mixture of II 10, 4'-(2-ethoxypropyloxy)**phenyl** p-decyloxybenzoate 50, and 4'-(4-methylhexyloxy)**phenyl** p-decyloxybenzoate 50 weight parts was sealed in a cell and cooled at 0.5°/h from its isotropic phase to 20°. The liquid crystal composition had 325 and 245 μs in response time at 10 and 30°, resp.

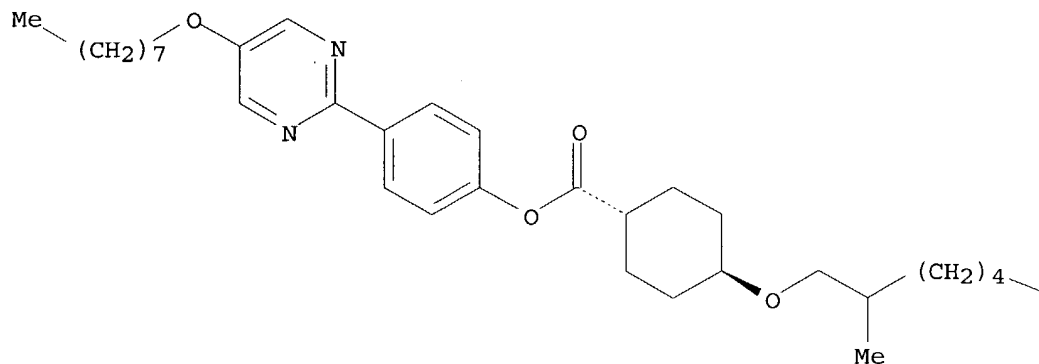
IT **117907-26-3**  
 RL: TEM (Technical or engineered material use); USES (Uses)  
 (liquid crystal compns. containing, for electrooptical display devices)  
 RN 117907-26-3 CAPLUS  
 CN Cyclohexanecarboxylic acid, 4-[(2-methylheptyl)oxy]-, 4-[5-(octyloxy)-2-

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pyrimidinylphenyl ester, trans- (9CI) (CA INDEX NAME)

Relative stereochemistry.

PAGE 1-A



PAGE 1-B

Me

L11 ANSWER 69 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1987:449772 CAPLUS  
DOCUMENT NUMBER: 107:49772  
TITLE: Smectic liquid-crystal phases  
INVENTOR(S): Hopf, Reinhard; Scheuble, Bernhard; Waechtler, Andreas; Hittich, Reinhard; Eidenschink, Rudolf; Geelhaar, Thomas; Krause, Joachim; Reiffenrath, Volker  
PATENT ASSIGNEE(S): Merck Patent G.m.b.H., Fed. Rep. Ger.  
SOURCE: PCT Int. Appl., 103 pp.  
CODEN: PIXXD2  
DOCUMENT TYPE: Patent  
LANGUAGE: German  
FAMILY ACC. NUM. COUNT: 2  
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 8701717	A2	19870326	WO 1986-EP529	19860915
WO 8701717	A3	19870521		
W: JP, KR, NO, US				
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
DE 3533333	A1	19870326	DE 1985-3533333	19850918
DE 3608500	A1	19870924	DE 1986-3608500	19860314

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WO 8705618            A1    19870924            WO 1986-EP513            19860905  
W: JP, KR, US  
RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE  
EP 259346            A1    19880316            EP 1986-905771            19860905  
EP 259346            B1    19900404  
R: CH, DE, FR, GB, LI, SE  
JP 63502657            T2    19881006            JP 1986-505063            19860905  
JP 63500948            T2    19880407            JP 1986-504895            19860915  
JP 2777885            B2    19980723  
DD 249707            A5    19870916            DD 1986-294526            19860918  
US 4886620            A    19891212            US 1987-51120            19870513  
NO 8702040            A    19870515            NO 1987-2040            19870515

PRIORITY APPLN. INFO.:

DE 1985-3533333            19850918  
DE 1986-3608500            19860314  
WO 1986-EP513            19860905  
WO 1986-EP529            19860915

AB    Comps. having neg. dielec. anisotropy for chiral smectic liquid-crystal phases used in electrooptical display devices are described. A liquid-crystal phase containing 4-(5-heptylpyrimidin-2-yl)**phenyl** (p-pentylbenzyl) ether 25, 4-(5-heptylpyrimidin-2-yl)**phenyl** (p-hexylbenzyl) ether 33, 4-(5-nonylpyrimidin-2-yl)**phenyl** (p-pentylbenzyl) ether 12, 4-(5-nonylpyrimidin-2-yl)**phenyl** (p-hexylbenzyl) ether 3, 2-p-nonyloxyphenyl-5-nonylpyrimidine 21, 2,3-dicyano-1,4-bis(trans-4-propylcyclohexylcarboxy)benzene 3, and 2,3-dicyano-1,4-bis(trans-4-pentylcyclohexylcarboxy)benzene 3% had crystalline-smectic C, smectic C-nematic, and nematic-isotropic phase transitions at 7, 64, and 95.5°, resp., and dielec. anisotropy -0.5.

IT    109203-83-0

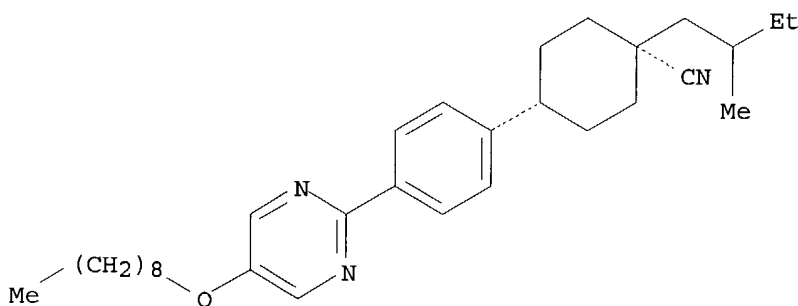
RL: USES (Uses)

(smectic liquid-crystal comps. containing, for display devices)

RN    109203-83-0    CAPLUS

CN    Cyclohexanecarbonitrile, 1-(2-methylbutyl)-4-[4-[5-(nonyloxy)-2-pyrimidinyl]phenyl]-, cis- (9CI)    (CA INDEX NAME)

Relative stereochemistry.



L11 ANSWER 70 OF 74    CAPLUS    COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER:            1981:443037    CAPLUS

DOCUMENT NUMBER:            95:43037

TITLE:                        Synthesis of 2,4-substituted 6,7-phenanthreno- and 6,7-acenaphthenopteridines

AUTHOR(S):                    Ram, Vishnu J.; Pandey, Hrishi Kesh; Vlietinck, Arnold J.

CORPORATE SOURCE:            Dep. Chem., S. C. Coll., Ballia, India

SOURCE:                      Journal of Heterocyclic Chemistry (1981), 18, 55-7

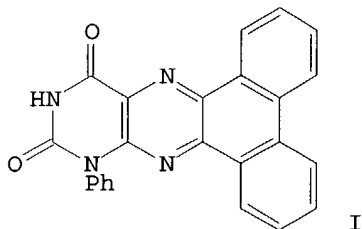
CODEN: JHTCAD; ISSN: 0022-152X

DOCUMENT TYPE:                Journal

LANGUAGE:                      English

09/ 811,359

OTHER SOURCE(S) : CASREACT 95:43037  
GI



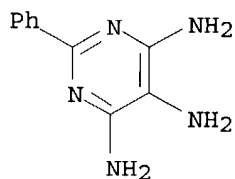
AB A series of 2- and 4-substituted 6,7-phenanthreno- and 6,7-acenaphthenopteridines were prepared. The structures of the compounds were confirmed by spectroscopic studies and elemental analyses. Thus, 1-phenyl-2,4-dioxo-5,6-diaminopyrimidine was treated with phenanthroquinone to give the phenanthrenopyrimidopyrazine I.

IT 78270-90-3

RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclization of, with phenanthraquinone and acenaphthone)

RN 78270-90-3 CAPLUS

CN 4,5,6-Pyrimidinetriamine, 2-phenyl- (9CI) (CA INDEX NAME)



L11 ANSWER 71 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1977:120945 CAPLUS

DOCUMENT NUMBER: 86:120945

TITLE: Synthesis and effect of some adamantane derivatives on the Sindbis virus

AUTHOR(S): Danilenko, G. I.; Vladimirtsev, I. F.; Yurchenko, A. G.; Galegov, G. A.; Leont'eva, N. O.; Isaev, S. D.; Dikolenko, E. I.; Boldyrev, I. V.; Yurchenko, R. I.; Kotenko, S. I.

CORPORATE SOURCE: Inst. Org. Chem., Kiev, USSR

SOURCE: Farmatsevtichnii Zhurnal (Kiev) (1976), (5), 36-40

CODEN: FRZKAP; ISSN: 0367-3057

DOCUMENT TYPE: Journal

LANGUAGE: Ukrainian

OTHER SOURCE(S): CASREACT 86:120945

AB 1-(4-Tolyl)- and 1-(4-anisyl)adamantane-3-carboxylic acids reacted with  $\text{PCl}_5$  in refluxing  $\text{CCl}_4$  and were treated with 25% aqueous  $\text{NH}_3$  to give the respective amides, which were treated with  $\text{NaOMe}$  in  $\text{MeOH}$  and then with  $\text{Br}$  to give the corresponding 3-[(N-methoxycarbonyl)amino]adamantanes. Treating adamantane-1-carbonyl chloride with 9 amines (e.g., 2-, 3-, and 4- $\text{MeOC}_6\text{H}_4\text{NH}_2$ , piperidine, 4,6-dichloropyrimidine) afforded the respective amides; those derived from primary and from  $\text{Et}_2\text{NH}$  were active against Sindbis virus reproduction, as were 1-(N-methacryloylamino)adamantane and its copolymer with (diethylamino)ethyl N-methacryloylanthranilate-HCl. (Adamantoylmethylene)triphenylphosphorane cyclized with  $\text{RN}_3$  ( $\text{R} = \text{Ph}$ , 4- $\text{O}_2\text{NC}_6\text{H}_4$ ) to give 72-83% 5-(1-adamantyl)-1-aryl-1,2,3-triazoles.

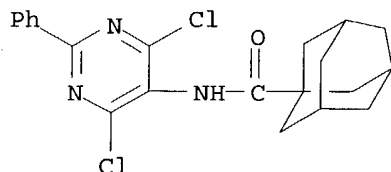
09/ 811,359

IT 62248-28-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)  
(preparation and virucidal activity of)

RN 62248-28-6 CAPLUS

CN Tricyclo[3.3.1.1<sup>3,7</sup>]decane-1-carboxamide, N-(4,6-dichloro-2-phenyl-5-pyrimidinyl)- (9CI) (CA INDEX NAME)



L11 ANSWER 72 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1976:107079 CAPLUS

DOCUMENT NUMBER: 84:107079

TITLE: Polycyclic dyes

INVENTOR(S): Dehnert, Johannes; Dunkelmann, Guenter

PATENT ASSIGNEE(S): BASF A.-G., Fed. Rep. Ger.

SOURCE: Ger. Offen., 26 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2430565	A1	19760115	DE 1974-2430565	19740626
DE 2430565	B2	19771027		
GB 1504532	A	19780322	GB 1975-21447	19750520
CH 612212	A	19790713	CH 1975-8141	19750623
FR 2276358	A1	19760123	FR 1975-19708	19750624
JP 51018735	A2	19760214	JP 1975-78684	19750626

PRIORITY APPLN. INFO.: DE 1974-2430565 19740626

GI For diagram(s), see printed CA Issue.

AB Seven polycyclic dyes (I, R = H, Cl; R1 = H, NO<sub>2</sub>; R2 = NH<sub>2</sub>, NH<sub>2</sub>t, NHCH<sub>2</sub>CH<sub>2</sub>OH, NMeCH<sub>2</sub>CH<sub>2</sub>OH, Me, NHCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>OMe, NHCH<sub>2</sub>CH<sub>2</sub>OCH<sub>2</sub>CH<sub>2</sub>OH; R3 = Ph, p-ClC<sub>6</sub>H<sub>4</sub>, NBu<sub>2</sub>, Me) were prepared and dyed polyester fibers fast, brilliant greenish yellow to yellow shades. Thus, 3-amino-6-chloroindazole [16889-21-7] was diazotized, coupled with 2-phenyl -4,6-diaminopyrimidine [52644-22-1] to give the azo derivative (II) [58514-83-3], and II heated in a boiling HOAc-H<sub>2</sub>SO<sub>4</sub> mixture for 12 hr to give I (R = Cl, R1 = H, R2 = NH<sub>2</sub>, R3 = Ph) [58514-84-4]. The other I were similarly prepared

IT 58514-73-1

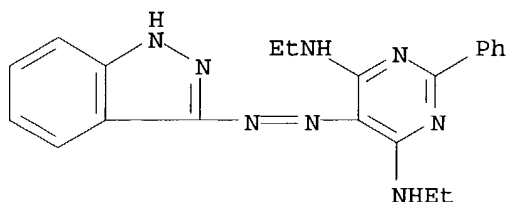
RL: RCT (Reactant); RACT (Reactant or reagent)  
(cyclization of)

RN 58514-73-1 CAPLUS

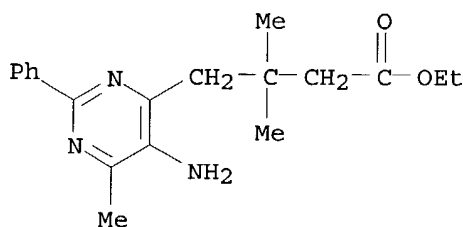
CN 4,6-Pyrimidinediamine, N,N'-diethyl-5-(1H-indazol-3-ylazo)-2-phenyl- (9CI)  
(CA INDEX NAME)



09/ 811,359



L11 ANSWER 73 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1973:526438 CAPLUS  
DOCUMENT NUMBER: 79:126438  
TITLE: 2-Oxo-4,4,9-trimethyl-7-phenyl  
-2,3,4,5-tetrahydro-(1H)-pyrimido[5,4-b] azepine  
AUTHOR(S): Strakov, A. Ya.; Brutane, D.  
CORPORATE SOURCE: Rizh. Politekh. Inst., Riga, USSR  
SOURCE: Latvijas PSR Zinatnu Akademijas Vestis, Kimijas Serija  
(1973), (2), 225-9  
CODEN: LZAKAM; ISSN: 0002-3248  
DOCUMENT TYPE: Journal  
LANGUAGE: Russian  
GI For diagram(s), see printed CA Issue.  
AB Pyrimidoazepinone (I) was prepared in 50% yield by heating quinazolone (II;  
X = O) with NaN<sub>3</sub> in polyphosphoric acid and in 90% yield by heating  
tosyloxime (II; X = NOSO<sub>2</sub>C<sub>6</sub>H<sub>4</sub>Me-p) in AcOH with Beckmann rearrangement.  
IT **50681-88-4P**  
RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)  
RN 50681-88-4 CAPLUS  
CN 4-Pyrimidinebutanoic acid, 5-amino-β,β,6-trimethyl-2-phenyl-,  
ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)



● HCl

L11 ANSWER 74 OF 74 CAPLUS COPYRIGHT 2004 ACS on STN  
ACCESSION NUMBER: 1967:403074 CAPLUS  
DOCUMENT NUMBER: 67:3074  
TITLE: Pteridinecarboxamide diuretics. II. Reaction of  
4,6-diamino-5-nitrosopyrimidines with N-substituted  
cyanoacetamides  
AUTHOR(S): Osdene, Thomas S.; Santilli, Arthur A.; McCardle, Lee  
E.; Rosenthale, Marvin E.  
CORPORATE SOURCE: Res. and Develop. Div., Wyeth Labs. Inc., Radnor, PA,  
USA  
SOURCE: Journal of Medicinal Chemistry (1967), 10(2), 165-7  
CODEN: JMCMAR; ISSN: 0022-2623  
DOCUMENT TYPE: Journal

09/ 811,359

LANGUAGE: English

GI For diagram(s), see printed CA Issue.

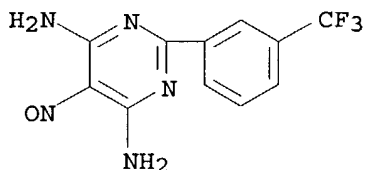
AB cf. CA 65: 12204g. Several new 4,6-diamino-2-substituted 5-nitrosopyrimidines and N-substituted 2-cyanoacetamides were prepared and used as intermediates in the base-catalyzed preparation of a number of 4,7-diamino-2-substituted N-substituted 6-pteridinecarboxamides as shown. Many of these pteridines had diuretic activity in rats after oral administration. Increased activity was associated with certain specific structural characteristics. The more active compds. were those in which the 2 position of the pteridine nucleus bears an aromatic group, preferably **phenyl** or m-chlorophenyl, and in which the carbamoyl N bears a 2-dialkylaminoethyl or 2-(N-heterocyclic amino)ethyl group, e.g., 2-diethylaminoethyl or 2-morpholinoethyl.

IT **15059-97-9P**

RL: SPN (Synthetic preparation); PREP (Preparation)  
(preparation of)

RN 15059-97-9 CAPLUS

CN Pyrimidine, 4,6-diamino-5-nitroso-2-( $\alpha,\alpha,\alpha$ -trifluoro-m-tolyl)- (8CI) (CA INDEX NAME)



=> d his

(FILE 'HOME' ENTERED AT 10:41:35 ON 21 FEB 2004)

FILE 'REGISTRY' ENTERED AT 10:41:51 ON 21 FEB 2004

L1 STRUCTURE UPLOADED

L2 STRUCTURE UPLOADED

L3 STRUCTURE UPLOADED

L4 8401 S L1 FUL

L5 5166 S L2 FUL

L6 316 S L3 FUL

FILE 'CAPLUS' ENTERED AT 10:45:05 ON 21 FEB 2004

L7 1933 S L4 OR L5

L8 878 S L7 NOT (PYRIDYL OR PYRIDIN? OR PYRIMIDIN? OR PYRIMIDYL OR PYR

L9 81 S L8 AND (PHENYL OR NAPHTHYL)

L10 68 S L6

L11 74 S L9 NOT L10